AR201-14132

Sarah_Loftus@americanchemistry.com on 12/16/2002 03:43:19 PM

To: Rtk Chem/DC/USEPA/US@EPA, oppt.ncic@epamail.epa.gov
cc:

Subject: HERTG HPV Submission - arylpolyolefins

HPV Test Plan Submission from the American Chemistry Council Petroleum Additives HERTG - HPV Registration Number

Three documents (1. cover letter, 2. test plan and 3. robust summaries) are attached to this e-mail for the HERTG HPV Arylpolyolefins. If you have any questions or comments, please feel free to contact me. Below, my contact information is listed. Thank you very much. Sarah McLallen

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(See attached file: Group 2.zip)

Group 2.zip

December 16, 2002

By Mail
Christine Todd Whitman, Administrator
US EPA
PO Box 1473
Merrifield, VA 22116

Attn: Chemical Right-to-Know Program – Test Plan Submission from HERTG
Registration Number

Dear Administrator Whitman:

The American Chemistry Council Petroleum Additives Panel (Panel) Health, Environmental, and Regulatory Task Group (HERTG) submits for review and public comment its test plan report, as well as related robust summaries, for the *"Arylpolyolefins"* under the Environmental Protection Agency's High Production Volume (HPV) Chemical Challenge Program. The HERTG understands that there will be a 120-day review period for the test plan report and that all comments generated by or provided to EPA will be forwarded to the HERTG for consideration.

Arylpolyolefins have a wide range of uses, but they are often employed as non-isolated intermediates for conversion to alkaryl sulfonates. Other uses of arylpolyolefins include use as base fluids in engine oils, transmission fluids, gear oils, hydraulic fluids and other lubricant fluid applications that require fluidity at low temperatures. Based upon the data reviewed in the attached report, the HERTG concludes that the physicochemical and toxicological properties of the proposed arylpolyolefins group are similar and follow a regular pattern as a result of structural similarity. The two chemicals in the arylpolyolefins group are as follows:

- Benzene, C_{14}-C_{24}-branched and linear alkyl derivatives (CAS # 115733-08-9) referred to in this report as the "C_{14}-C_{24} alkaryl derivative."
- Benzene, polypropene derivatives (CAS # 68081-77-6) referred to in this report as the "polypropene derivative."

Below, the test plan for the arylpolyolefins is briefly summarized.

- Water solubility – Solubility data will be developed for the C_{14}-C_{24} alkaryl derivative (CAS # 115733-08-9) and will be used to characterize the water solubility of the other category

member. The C_{14}-C_{24} alkaryl derivative (CAS # 115733-08-9) is the lower molecular weight category member and likely to have the highest water solubility.

- Biodegradation - Biodegradation data will be developed for the C_{14}-C_{24} alkaryl derivative (CAS # 115733-08-9) and will be used to characterize the biodegradability of the other category member. The C_{14}-C_{24} alkaryl derivative (CAS # 115733-08-9) is the lower molecular weight, more water-soluble category member and has the potential to exhibit the greatest extent of biodegradability.
- Aquatic Toxicity – Acute toxicity testing with a freshwater fish, invertebrate and alga will be conducted on the C_{14}-C_{24} alkaryl derivative (CAS # 115733-08-9) and will be used to characterize the aquatic toxicity of the other category member.
- Mutagenicity – An *in vitro* chromosomal aberration study will be conducted on the C_{14}-C_{24} alkaryl derivative (CAS # 115733-08-9) and the results will be bridged to the other category member.
- Systemic toxicity – An oral repeated-dose toxicity study will be conducted on the C_{14}-C_{24} alkaryl derivative (CAS # 115733-08-9) and the results will be bridged to the other category member.
- Reproductive/developmental toxicity – A reproductive/developmental toxicity study will be conducted on the C_{14}-C_{24} alkaryl derivative (CAS # 115733-08-9) and the results will be bridged to the other category member.

As this test plan was developed, careful consideration was given to the number of animals that would be required for tests included in the proposed plan and conditions to which the animals might be exposed. In consideration of the concerns of some non-governmental organizations about animal welfare, the use of animals in this proposed test plan has been minimized.

Thank you in advance for your attention to this matter. If you have any questions regarding the test plan report or the robust summaries, or HERTG's activities associated with the Challenge Program, please contact Sarah McLallen at 703-741-5607 (telephone), 703-741-6091 (telefax) or Sarah_McLallen@americanchemistry.com (e-mail).

Sincerely yours,

Courtney M. Price
Vice President, CHEMSTAR

cc: HERTG members

AR201-14132A

HIGH PRODUCTION VOLUME (HPV)

CHEMICAL INITIATIVE

Analysis Document and Testing Plan

For

ARYLPOLYOLEFINS

Prepared by
The American Chemistry Council
Petroleum Additives Panel
Health, Environmental, and Regulatory Task Group

November 26, 2002

Group 2 - ARYLPOLYOLEFIN
November 26, 2002

LIST OF MEMBER COMPANIES IN THE HEALTH, ENVIRONMENTAL AND REGULATORY TASK GROUP

The Health, Environmental, and Regulatory Task Group (HERTG) of the American Chemistry Council Petroleum Additives Panel includes the following member companies:

B.P. plc

Chevron Oronite Company, LLC

Crompton Corporation

Ethyl Corporation

ExxonMobil Chemical Company

Ferro Corporation

Infineum

The Lubrizol Corporation

Rhein Chemie Corporation

Rhodia, Inc.

EXECUTIVE SUMMARY

The American Chemistry Council Petroleum Additives Panel Health, Environmental, and Regulatory Task Group (HERTG), and its member companies, hereby submit for review this category analysis document and testing plan for the *"arylpolyolefins"* under the International Council of Chemical Associations (ICCA) Initiative on High Production Volume (HPV) chemicals. This report should be read in its entirety in order to obtain a complete understanding of the category and proposed testing.

Arylpolyolefins. Relying on several factors specified in the OECD guidance document on "Development of Chemical Categories in the HPV Challenge Program," in which use of chemical categories is encouraged, the following two closely related high production volume chemicals are submitted as a category:

- Benzene, C_{14}-C_{24}-branched and linear alkyl derivatives (CAS # 115733-08-9) referred to in this report as the "C_{14}-C_{24} alkaryl derivative."
- Benzene, polypropene derivatives (CAS # 68081-77-6) referred to in this report as the "polypropene derivative."

Structural Similarity. A key factor that supports these chemicals as a category is their structural similarity. The two category members are composed of chemical constituents that contain one aromatic ring to which an alkyl group is attached. The alkyl group is either linear or methyl branched and ranges in carbon (C) number from C_{14} to approximately C_{82}.

Similarity of Physicochemical Properties. The physicochemical properties of these substances are generally similar or overlap and can be explained by their similarities in chemical structure and chemical processing. They are clear to yellow-colored liquids at ambient temperatures and have high boiling points. These substances have low volatility due to their low vapor pressure and relatively high molecular weights. Arylpolyolefins have low water solubility and have high Kow values.

Fate and Transport Characteristics. The potential of the members of the arylpolyolefin category to biodegrade varies in accordance with their chemical structure. Category members with linear alkyl side chains are expected to biodegrade to a high extent, but category members with branched alkyl side chains are expected to have a limited potential to biodegrade. Since members of this category have low water solubility, hydrolysis testing is technically unfeasible. Furthermore, category members are resistant to hydrolysis because they lack hydrolyzable moieties. Component molecules of category members do not absorb sufficient light energy to result in a structural transformation, therefore they are not subject to direct photolytic reactions. Although arylpolyolefins have a low potential to partition to the air to a significant degree because of their low vapor pressure, computer-modeled data characterizing the atmospheric oxidation potential (indirect photodegradation) for category members suggest that they will degrade rapidly in air. These substances are not expected to partition to water or air if released

into the environment due to their low water solubility and low vapor pressure, and partitioning data suggest that chemical components of category members will partition primarily to soil.

Toxicological Similarity. Review of existing published and unpublished test data for members of this category shows predominantly low mammalian toxicity as discussed below.

Aquatic Toxicology. Aquatic toxicity data are not available to characterize category members. Therefore, data will be developed to characterize the fish, invertebrate and alga toxicity of category members.

Mammalian Toxicology - Acute. Data on acute mammalian toxicity were reviewed. The findings indicate a low degree of acute toxicity. Data are available for both members of the arylpolyolefin category indicating that the category has been well tested for acute mammalian effects. Therefore, no additional acute mammalian toxicity testing is necessary.

Mammalian Toxicology - Genotoxicity. An *in vitro* bacterial gene mutation assay was reviewed for the C_{14}-C_{24} alkaryl derivative (CAS # 115733-08-9). The C_{14}-C_{24} alkaryl derivative (CAS # 115733-08-9) did not demonstrate mutagenic activity in either the presence or absence of metabolic activation. This test will be used for bridging to the other category member. No chromosomal aberration assays are available for the members of the arylpolyolefin category. It is recommended that an *in vitro* chromosomal aberration assay be conducted for the C_{14}-C_{24} alkaryl derivative (CAS # 115733-08-9) and the results bridged to the other category member.

Mammalian Toxicology - Subchronic Toxicity. There are no repeated-dose toxicity studies available for the members of the arylpolyolefin category. It is recommended that an oral repeated-dose toxicity study be conducted for the C_{14}-C_{24} alkaryl derivative (CAS # 115733-08-9) and the results bridged to the other category member.

Mammalian Toxicology - Reproductive and Developmental Toxicity. There are no reproductive or developmental toxicity studies available for the members of the arylpolyolefin category. It is recommended that a reproductive/developmental toxicity study be conducted for the C_{14}-C_{24} alkaryl derivative (CAS # 115733-08-9) and the results bridged to the other category member.

Conclusion. Based upon the data reviewed for this category analysis document, it is concluded that the existing physicochemical and toxicological properties of the arylpolyolefins are similar or overlap as a result of their structural relatedness. Thus, these chemicals are considered to constitute a category and additional data will be developed in accordance with the arylpolyolefin test plan summarized below.

Testing Plan. The test plan for the arylpolyolefin category includes the following:

- Water solubility – Solubility data will be developed for the C_{14}-C_{24} alkaryl derivative (CAS # 115733-08-9) and will be used to characterize the water solubility of the other category

member. The C_{14}-C_{24} alkaryl derivative (CAS # 115733-08-9) is the lower molecular weight category member and likely to have the highest water solubility.

- Biodegradation - Biodegradation data will be developed for the C_{14}-C_{24} alkaryl derivative (CAS # 115733-08-9) and will be used to characterize the biodegradability of the other category member. The C_{14}-C_{24} alkaryl derivative (CAS # 115733-08-9) is the lower molecular weight, more water-soluble category member and has the potential to exhibit the greatest extent of biodegradability.
- Aquatic Toxicity – Acute toxicity testing with a freshwater fish, invertebrate and alga will be conducted on the C_{14}-C_{24} alkaryl derivative (CAS # 115733-08-9) and will be used to characterize the aquatic toxicity of the other category member.
- Mutagenicity – An *in vitro* chromosomal aberration study will be conducted on the C_{14}-C_{24} alkaryl derivative (CAS # 115733-08-9) and the results will be bridged to the other category member.
- Systemic toxicity – An oral repeated-dose toxicity study will be conducted on the C_{14}-C_{24} alkaryl derivative (CAS # 115733-08-9) and the results will be bridged to the other category member.
- Reproductive/developmental toxicity – A reproductive/developmental toxicity study will be conducted on the C_{14}-C_{24} alkaryl derivative (CAS # 115733-08-9) and the results will be bridged to the other category member.

As this test plan was developed, careful consideration was given to the number of animals that would be required for tests included in the proposed plan and conditions to which the animals might be exposed. In consideration of the concerns of some non-governmental organizations about animal welfare, the use of animals in this proposed test plan has been minimized.

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1.0 INTRODUCTION

In March 1999, the American Chemistry Council (formerly the Chemical Manufacturers Association) Petroleum Additives Panel - Health, Environmental, and Regulatory Task Group (HERTG) and its participating member companies committed to address for certain chemicals listed under the United States Environmental Protection Agency (EPA) High Production Volume (HPV) Chemical Challenge Program and the International Council of Chemical Associations (ICCA) Initiative on HPV chemicals. This category analysis document and testing plan follows up on that commitment.

Specifically, this category analysis document and testing plan sets forth how the HERTG intends to address relevant physicochemical, environmental, aquatic and health effects information for the following substances:

- Benzene, C_{14}-C_{24}-branched and linear alkyl derivatives (CAS # 115733-08-9) referred to in this report as the "C_{14}-C_{24} alkaryl derivative."
- Benzene, polypropene derivatives (CAS # 68081-77-6) referred to in this report as the "polypropene derivative."

An analysis of the available data on these chemicals supports the designation of the arylpolyolefins as a "chemical category" as provided in the OECD guidance document entitled, "Development of Chemical Categories in the HPV Challenge Program". This category analysis document provides the basis for that determination, indicates the findings of the data review process, and sets forth a proposed test plan to satisfy parts of the required test battery for endpoints without data that would be considered adequate under the Initiative.

The United States EPA guidance on the HPV Program indicates that the primary purpose of the program is to encourage "the chemical industry . . . to voluntarily compile a Screening Information Data Set (SIDS) on all chemicals on the HPV list" (EPA, "Development of Chemical Categories in the HPV Challenge Program," p. 1). The ICCA HPV Chemical Initiative has the same primary purpose for all chemicals on the ICCA HPV lists. At the same time, both the ICCA and EPA recognize that the "large number of chemicals to be tested makes it important to reduce the number of tests to be conducted, *where this is scientifically justifiable.*" (*Id.*, p. 1) [emphasis added] The next part of the EPA guidance explains where this would be scientifically justifiable:

> One approach is to test closely related chemicals as a group, or category, rather than test them as individual chemicals. In the category approach, *not every chemical needs to be tested for every SIDS endpoint.* However, *the test data finally compiled* for the category must prove adequate to support a screening level hazard-assessment of the category and its members. That is, the *final data set* must allow one to estimate the hazard for the untested endpoints, *ideally* by interpolation between and among the category members. In certain cases, where toxicity is low and no upward trend is expected, extrapolation to the higher category members may be acceptable. (*Id.*, p. 1) [emphasis added].

EPA guidance goes on to state, "The use of categories is encouraged in the Challenge Program and will have a number of benefits." (*Id.*, p. 1) Among the benefits identified in the guidance for the use of categories are "a reduction in testing will result in fewer animals used to test a category of chemicals as opposed to doing each test on each individual chemical," and "there will be . . . economic savings since less testing may be needed for chemicals considered as a category." (*Id.*, p. 1) That guidance also states that categories "accomplish the goal of the Challenge Program – to obtain screening level hazard information – through the strategic application of testing to the category." (*Id*, p. 2)

A similarly stated intent "to reduce the number of tests to be conducted, *where this is scientifically justifiable*" was articulated by the EPA in its draft guidance document titled, "The Use of Structure Activity Relationships (SAR) in the High Production Volume Chemicals Challenge Program." [emphasis added].

The EPA "Chemical Categories" guidance defines a "chemical category" as a group of chemicals whose physicochemical and toxicological properties *are likely to* be similar *or* follow a regular pattern as a result of structural similarity." (*Op. Cit.*, p. 2) [emphasis added].

According to the guidance, what is important is that the "structural similarities [among members of the group] *may* create a predictable pattern *in any* or all of the following parameters: physicochemical properties, environmental fate, aquatic effects, and human health effects." (Id., p. 2) [emphasis added]. Thus, it is not necessary for the chemicals in a category to be similar in all respects. Nor must there be conclusive proof that the chemicals in the postulated category will behave identically across all relevant parameters. All that is required for an acceptable category is that there be a *likelihood* of similarity of physicochemical and toxicological properties or a *likelihood* that the chemicals will in some pertinent respect follow a regular pattern as a result of their structural similarity.

In identifying the arylpolyolefin category, the six-step process set out in the EPA guidance on category development was followed. As the information below indicates, the arylpolyolefin category of chemicals clearly satisfies the standards established in that guidance for use of a chemical category:

Step 1: group structurally similar chemicals into a putative category

Step 2: gather relevant published and unpublished literature for each member of the category

Step 3: evaluate the compiled data for adequacy in accordance with the EPA guidance documentation

Step 4: construct matrices of SIDS endpoints versus category members arranged so as to indicate the structural progression of the category (in this case, by increasing molecular weight)

Step 5: evaluate the data to determine whether there is a correlation between category members for each SIDS endpoint

Step 6: make available, to the ICCA and the public, this test plan including the foregoing category rationale and the following data assessment with the proposed testing scheme for the arylpolyolefins.

2.0 CHEMISTRY OF ARYLPOLYOLEFINS

2.1 DESCRIPTION

Arylpolyolefins consist of a benzene ring with one long-chain alkyl substituent group. The alkyl group is a saturated hydrocarbon chain that can vary in length and extent of branching. The chemical names and CAS numbers for the members of the category are presented in Table 1 and the chemical structures are presented in Table 2.

Commercial arylpolyolefins are manufactured by reacting anhydrous alkylate (linear or branched) with benzene in the presence of catalyst and heat. Linear alkylbenzenes use linear alpha olefins with $AlCl_3$ and HF as the preferred catalyst. Branched alkylbenzenes start with a tetrapropenyl (C_3) stream using HF as the preferred catalyst, but triethyl aluminum ($AlEt_3$) has also been used as a catalyst.

2.2 PHYSICOCHEMICAL PROPERTIES

Selected physicochemical properties of arylpolyolefin category members are presented in Table 3. The physicochemical properties of these two substances are generally similar or overlap, as would be expected based upon the similarity in their chemical structure and chemical processing, and thus support consideration of these substances as a category.

2.2.1 Molecular Weight and Alkyl Side Chain Length

The category members range in molecular weight from 275 to 415 daltons for the C_{14}-C_{24} alkaryl derivative (CAS # 115733-08-9) and 387 to 1228 daltons for the polypropene derivative (CAS # 68081-77-6) (Table 3). The structural variable that is responsible for the range in molecular weight of the category members is the number of carbon atoms in the alkyl chain on the benzene ring.

2.2.2 Specific Gravity

The specific gravity of category members are 0.85 for the C_{14}-C_{24} alkaryl derivative (CAS # 115733-08-9) and 0.87 for the polypropene derivative (CAS # 68081-77-6) (Table 3).

2.2.3 Viscosity

The viscosity of category members are 21 cSt @ 40°C for the C_{14}-C_{24} alkaryl derivative (CAS # 115733-08-9) and 93 cSt @ 40°C for the polypropene derivative (CAS # 68081-77-6) (Table 3).

2.2.4 Melting Point

The category members are viscous liquids at ambient temperatures.

2.2.5 Boiling Point

Modeling data[1] indicate that the boiling range of category members can range from 342 to 458°C for the C_{14}-C_{24} alkaryl derivative (CAS # 115733-08-9) and can be >388°C for the polypropene derivative (CAS # 68081-77-6) (Table 3).

The modeling data for physicochemical endpoints in Sections 2.2.5 to 2.2.7 are presented as ranges for category members, where possible, and are based on the highest and lowest molecular weight derivative in each member. For example, structures representing the C_{14}-C_{24} alkaryl derivative (CAS # 115733-08-9) include a benzene C_{14} alkyl derivative and a benzene C_{24} alkyl derivative. Whereas, structures representing the polypropene derivative (CAS # 68081-77-6) include only the benzene C_{22} polypropene lowest molecular weight derivative; the benzene C_{82} polypropene highest molecular weight derivative has not been modeled as the molecular weight of this derivative falls outside of the applicable range of the EPIWIN modeling program. The idealized structures are shown in Table 2. The physicochemical information used in the modeling is found in Table 3.

2.2.6 Vapor Pressure

Modeling data indicate that the vapor pressure range of category members can range from $1.3e^{-2}$ to $1.7e^{-6}$ Pa at 25 °C for the C_{14}-C_{24} alkaryl derivative (CAS # 115733-08-9) and can be $<6.2e^{-4}$ Pa at 25 °C for the polypropene derivative (CAS # 68081-77-6) (Table 3).

2.2.7 Water Solubility and Octanol-Water Partition Coefficients

Modeling data indicate that the water solubility range of category members can range from $2.0e^{-4}$ to $4.4e^{-9}$ mg/L at 25 °C for the C_{14}-C_{24} alkaryl derivative (CAS # 115733-08-9) and can be $<1.2e^{-7}$ mg/L at 25 °C for the polypropene derivative (CAS # 68081-77-6). The low water solubility is consistent with the high lipophilic nature and high molecular weight of these substances. Modeling data indicate that the log of the octanol-water partition coefficients (log K_{ow}) for category members are estimated to be >8.9.

The water solubility of category members will be characterized by conducting a water solubility test with the C_{14}-C_{24} alkaryl derivative (CAS # 115733-08-9). The data developed for this substance will be used to estimate the water solubility of the polypropene derivative (CAS # 68081-77-6).

3.0 USES OF ARYLPOLYOLEFINS

Arylpolyolefins have a wide range of uses, but they are often employed as non-isolated intermediates for conversion to alkaryl sulfonates (HERTG-HPV Group 3). Other uses of arylpolyolefins include use as base fluids in engine oils, transmission fluids, gear oils, hydraulic fluids and other lubricant fluid applications that require fluidity at low temperatures. Some arylpolyolefins are also used as refrigerant lubricants and thermal transfer fluids.

4.0 EVALUATION OF AVAILABLE PUBLIC AND COMPANY DATA

4.1 Environmental Fate Data

4.1.1 Physicochemical Properties Relevant to Environmental Fate

In order to evaluate the environmental fate of a substance, it is important to understand its potential degradability and partitioning behavior among environmental compartments (i.e., air, soil, sediment, suspended sediment, water and biota).

The physicochemical properties and molecular structure of a chemical will influence the degradation processes it may be subjected to in the environment. Potentially important environmental degradation pathways include biodegradation, hydrolysis and photodegradation. Biodegradation of an organic chemical by bacteria can provide energy and carbon for microbial growth. This process results in a structural change of the chemical. Biodegradation can result in the complete loss of an organic chemical, producing carbon dioxide, mineral salts and water. Hydrolysis is a reaction in which a water molecule or hydroxide ion substitutes for another atom or group of atoms present in an organic chemical resulting in a structural change of that chemical. Chemical photodegradation results in a structural change of a molecule from the absorption of solar radiation.

The physicochemical properties of a substance will also influence the way in which it partitions among environmental compartments (i.e., air, water, soil and sediment). Generally, substances characterized by a low vapor pressure do not partition into air to a great extent. Similarly, substances characterized by a low water solubility do not partition

extensively into water. Substances that do not partition into air and water to any great extent tend to partition into soil and sediments.

4.1.2 Biodegradability

4.1.2.1 Testing Methodologies

The potential biodegradability of a substance in water, under aerobic conditions can be assessed using one of the OECD 301 testing guidelines. Chemical biodegradation involves a series of microbial-mediated reactions that can require many different microorganisms acting together to degrade a parent substance. There are several standard test methods that measure primary degradation (i.e., loss of parent chemical) or ultimate degradation (i.e., complete utilization of a substance to produce carbon dioxide, water, mineral salts and microbial biomass). Primary degradation can be determined analytically by measuring dissolved organic carbon (DOC) for water-soluble chemicals, infrared absorbance, or by a chemical-specific detection method. Ultimate degradation (also called mineralization), as mediated by microorganisms, can be determined by measuring oxygen consumption or carbon dioxide evolution relative to the theoretical levels that can be derived based on an elemental analysis of the chemical under investigation.

4.1.2.2 Summary of Available Data

Biodegradation data are not available for members of the arylpolyolefin category. The first category member, the C_{14}-C_{24} alkaryl derivative (CAS # 115733-08-9), is expected to exhibit a higher extent of biodegradability in comparison to the second category member, the polypropene derivative (CAS # 68081-77-6). A lower extent of biodegradability is expected for the polypropene derivative (CAS # 68081-77-6) because of its higher molecular weight and subsequently lower anticipated water solubility. Low water solubility will limit availability to the degrading microorganisms and therefore will limit the potential extent of degradation possible within the guidelines and 28-day duration of a standard test procedure. Additionally, the degree of methyl branching along the alkyl group of the polypropene derivative (CAS # 68081-77-6) (Table 2) will also contribute to a reduced extent of degradation possible under a standard test procedure.

4.1.2.3 Data Assessment and Test Plan for Biodegradability

Biodegradation testing is proposed for the first category member, the C_{14}-C_{24} alkaryl derivative (CAS # 115733-08-9). The data developed for this substance will be used to estimate the biodegradability of the polypropene derivative (CAS # 68081-77-6).

4.1.3 Hydrolysis

4.1.3.1 Testing Methodologies

The potential for a substance to hydrolyze in water can be assessed as a function of pH (OECD Guideline 111, Hydrolysis as a Function of pH[1]). When an organic molecule undergoes hydrolysis, a nucleophile (water or hydroxide ion) attacks an electrophile and displaces a leaving group (e.g., halogen, phenoxide). Potentially hydrolyzable groups include alkyl halides, amides, carbamates, carboxylic acid esters and lactones, epoxides, phosphate esters and sulfonic acid esters[2]. The lack of a suitable leaving group renders compounds resistant to hydrolysis.

4.1.3.2 Summary of Available Data

Published or unpublished hydrolysis studies for members of the arylpolyolefin category are not available. Arylpolyolefins do not contain functional groups that are subject to hydrolytic reactions. Thus, these substances have little, if any, potential for hydrolysis and they are expected to be stable in water.

4.1.3.3 Data Assessment and Test Plan for Hydrolysis

Arylpolyolefins do not contain functional groups that are susceptible to hydrolytic degradative mechanisms. Therefore, testing these substances for hydrolysis is not needed to adequately evaluate this endpoint. A technical discussion for hydrolysis is presented as a robust summary.

4.1.4 Photodegradation

4.1.4.1 Testing and Modeling Methodologies

Photodegradation can occur as a result of direct and indirect mechanisms. Direct photodegradation can be measured in solution using the OECD test guideline 113. Indirect photodegradation can be estimated using a model accepted by the US EPA; this estimation method applies a calculation procedure to determine an atmospheric oxidation potential (AOP) value.

Direct photochemical degradation occurs through the absorbance of solar radiation by a chemical substance. If the absorbed energy is high enough, then the resultant excited state of the chemical may lead to its transformation. A prerequisite for direct photodegradation is the ability of one or more bonds within

[1] Organization for Economic Cooperation and Development (OECD) (1993) OECD Guidelines for Testing of Chemicals. OECD. Paris, France.
[2] W.J. Lyman, W.F. Reehl, and D.H. Rosenblatt. (1982) Handbook of Chemical Property Estimation Methods. McGraw-Hill Book Co. New York, NY, USA.

a chemical to absorb ultraviolet (UV)/visible light in the 290 to 750 nm range. Light wavelengths longer than 750 nm do not contain sufficient energy to break chemical bonds, and wavelengths below 290 nm are shielded from the earth by the stratospheric ozone layer. Indirect photodegradation also requires light energy as well as a series of chemical reactions that include the reaction of a molecule with hydroxyl radicals (OH-).

For estimation of indirect photodegradation, the computer program AOPWIN (atmospheric oxidation program for Microsoft Windows[3]) is used by the US EPA OPPTS (Office of Pollution Prevention and Toxic Substances). This program calculates a chemical half-life based on an overall OH- reaction rate constant, a 12-hour day and a specific OH- concentration.

4.1.4.2 Summary of Available Data

Published or unpublished direct photodegradation studies for the arylpolyolefin category members are not available. Review of the structures of arylpolyolefins indicates that they do not contain bonds that have a significant potential to absorb UV light above 290 nm. Therefore, the arylpolyolefins are not anticipated to undergo direct photodegradation.

Indirect photodegradation data (calculated AOP values) are available to characterize this endpoint for the arylpolyolefin category members (Table 4). Those data show that the parent chemical components of category members have a relatively short half-life in air, approximately 3 to 6 hours. However, given the low vapor pressure of these products, it is unlikely that this degradation process will contribute to their loss from the environment because the chemical components of these products will not tend to significantly partition to the air where this degradation process occurs. These data suggest that those chemical components that do partition to the air phase will degrade rapidly due to hydroxyl radical attack.

AOP values are presented as ranges for category members, where possible, and are based on the highest and lowest molecular weight derivative in each member. For example, structures representing the C_{14}-C_{24} alkaryl derivative (CAS # 115733-08-9) include a benzene C_{14} alkyl derivative and a benzene C_{24} alkyl derivative. Whereas, structures representing the polypropene derivative (CAS # 68081-77-6) include only the benzene C_{22} polypropene lowest molecular weight derivative; the benzene C_{82} polypropene highest molecular weight derivative has not been modeled as the molecular weight of this derivative falls outside of the applicable range of the EPIWIN modeling program.

[3] EPIWIN. 1999. Estimation Program Interface for Windows, version 3.04. Syracuse Research Corporation, Syracuse, NY, USA.

4.1.4.3 Data Assessment and Test Plan for Photodegradation

Based on their structures, arylpolyolefins are not anticipated to undergo direct photodegradation. Therefore, no additional testing for direct photodegradation is planned. A technical discussion for this endpoint is presented as a robust summary. For indirect photodegradation, calculated AOP values of selected chemical structures representative of the arylpolyolefin category members are available to characterize this endpoint. Therefore, no additional modeling is planned. The data suggest that the arylpolyolefin category members would be subject to rapid degradation in air from OH- attack. This effect would be limited by the low vapor pressure of these materials.

4.1.5 Fugacity Modeling

4.1.5.1 Modeling Methodologies

Fugacity-based multimedia fate modeling calculates the relative distribution of a chemical between environmental compartments. A widely used model for this approach is the EQC model[4].

There are multiple levels of the EQC model, which vary in complexity and data requirements. In the document, "Determining the Adequacy of Existing Data", EPA states that it accepts Level I fugacity modeling to estimate transport/distribution values. The EQC Level I model utilizes input of basic chemical properties, including molecular weight, vapor pressure and water solubility to calculate the percent distribution of a chemical within a standardized environment (unit world). Another EQC model, the Level III, uses these parameters, as well as chemical emission rates into air, water and soil and chemical degradation rates in air, water, soil and sediment.

4.1.5.2 Summary of Available Data

Published or unpublished fugacity data for the arylpolyolefin category members are not available. Arylpolyolefins have low vapor pressure and low water solubility, which suggests that they will not partition into the air or water to a great extent. Fugacity-based multimedia fate data for the arylpolyolefin category members suggest that these substances will partition to soil (Table 5).

Distribution values are presented as ranges for category members, where possible, and are based on the highest and lowest molecular weight derivative in each member. For example, structures representing the C_{14}-C_{24} alkaryl derivative (CAS # 115733-08-9) include a benzene C_{14} alkyl derivative and a benzene C_{24} alkyl

[4] Mackay, D., A. Di Guardo, S. Paterson, and C. E. Cowan. 1996. Evaluating the Environmental Fate of a Variety of Types of Chemicals Using the EQC Model. Environ. Toxicol. Chem. 15:1627-1637.

derivative. Whereas, structures representing the polypropene derivative (CAS # 68081-77-6) include only the benzene C_{22} polypropene lowest molecular weight derivative; the benzene C_{82} polypropene highest molecular weight derivative has not been modeled as the molecular weight of this derivative falls outside of the applicable range of the EPIWIN modeling program used to generate the physicochemical input data for the EQC Level I fugacity model.

4.1.5.3 Data Assessment and Test Plan for Fugacity

The relative distribution of substances within this category among environmental compartments was evaluated using the EQC Level I model (Table 5). Data developed using an EQC Level I model can be used for simple comparative purposes across several substances. The data suggest that category members will partition primarily to soil.

The EQC Level III model was not used for this evaluation because appropriate emission levels as yet are unknown. Because of the physical nature of the substances in this category, a Level I dataset was adequate to assess the potential partitioning behavior of arylpolyolefin category members in the environment.

Input data to run the EQC Level I model required an additional computer model to estimate selected physicochemical properties from a structure. The model used for this purpose was EPIWIN, version 3.04[5]. EPIWIN includes algorithms for estimating all physical and chemical properties needed for the EQC model.

4.2. ECOTOXICOLOGY DATA

4.2.1 Aquatic Ecotoxicity Testing

4.2.1.1 Test Methodologies

Acute aquatic ecotoxicity testing can include three species that represent three trophic levels in the freshwater aquatic environment: fish, invertebrates and algae. The fish acute toxicity test (OECD Guideline 203, *Fish, Acute Toxicity Test*) determines the lethality of a substance to a fish during a 96-hour exposure period. The invertebrate toxicity test (OECD Guideline 202, *Daphnia sp., Acute Immobilization Test and Reproduction Test*) determines the potential of a substance to immobilize an invertebrate, typically a daphnid (*Daphnia magna*), during a 48-hour exposure period. The alga growth inhibition test (OECD Guideline 201, *Alga, Growth Inhibition Test*) determines the potential of a substance to inhibit alga growth, typically using the freshwater unicellular green

[5] EPIWIN. 1999. Estimation Program Interface for Windows, version 3.04. Syracuse Research Corporation, Syracuse, NY, USA.

algae, *Pseudokirchneriella subcapitata* (formerly called *Selenastrum capricornutum*), during a 72-or 96-hour exposure period.

Three different exposure methodologies are available to conduct aquatic toxicity tests; i.e., flow-through, static and static renewal.

In *flow-through exposures*, organisms are exposed to a constant chemical concentration or loading in each treatment level in the incoming water and there is typically greater assurance than with other test methods that the exposure levels and water quality remains constant throughout the test. Although flow-through testing is a preferred method, it is most applicable for chemicals that have adequate water solubility.

In *static exposures*, organisms are exposed to a chemical in a test medium that is not replaced for the duration of the study. There is less assurance that the test material concentrations to which test organisms are exposed will remain constant because test material will have a greater opportunity to be lost from the aqueous phase by being adsorbed onto test chambers, degraded, volatilized, or otherwise changed during the test. Nevertheless, due to limitations of other test systems for non-volatile materials, the static test has been widely used and in some instances must be used, as is the case when conducting an alga test.

The *static-renewal exposure* is similar to a static exposure because it is conducted in still water, but the test solutions and control water are renewed periodically, usually every 24 hours. Daily test solution renewal provides a greater likelihood that the exposure concentrations or loadings will remain stable throughout the test. This is the preferred method for conducting fish toxicity tests for compounds such as the arylpolyolefins. Daily renewals cannot be done in the alga test, and dependent on the substance and test procedure used, renewals may not be possible for the *Daphnia* test because the process of exposure solution separation and replenishment can cause a discontinuity in the alga growth rate and it can stress *Daphnia* or result in coating or entrapping the organisms in surface film that may form during renewal operations, respectively. OECD considers the use of static testing for fish, *Daphnia* and algae and the use of static renewal testing for fish to be appropriate when evaluating the toxicity of complex, poorly water-soluble chemicals like arylpolyolefins, provided that test solution preparation uses water accommodated fraction or water soluble fraction preparation methods[6].

4.2.1.2 Test Solution Preparation

Arylpolyolefins are complex, poorly water-soluble substances, and it is not possible to prepare exposure solutions for aquatic toxicity testing by direct

[6] Organization for Economic Cooperation and Development (OECD) (2000). Guidance Document on Aquatic Toxicity Testing of Difficult Substances and Mixtures. OECD Environmental Health and Safety Publications, Series on Testing and Assessment No.23, Paris, France.

addition of measured quantities of test material to aqueous media. Two methods are used to prepare solutions of complex, poorly water-soluble materials for aquatic toxicity testing as recommended in the OECD guidance document on testing difficult substances[7]:

- *Water accommodated fraction* (WAF) – This is a method in which the test solution contains only that fraction of the test material (organic phase), which is retained in the aqueous phase after a period of stirring sufficient to reach equilibrium, followed by a sufficient time for phase separation. The WAF (aqueous phase) will contain soluble components of the test material at levels that will be dependent on the test material loading (the amount of material added to the aqueous medium). The resulting WAF is used in the aquatic toxicity test. Ideally, a WAF consists of a water-soluble extract of test material, but it can also include a stable micro-emulsion or contain small amounts of suspended matter.

- *Water soluble fraction* (WSF) – This is a method in which a WAF is either filtered, centrifuged, or allowed to settle for a greater length of time (24 hours) than with the WAF method, to remove suspended matter or emulsions from the aqueous phase before being used in the aquatic toxicity test.

4.2.1.3 Reporting Toxicity Results

In both WAF and WSF tests, test material exposures are expressed as loading rates (i.e., defined as the weight of test material added per unit volume of test medium during WAF or WSF preparation)[7]. For fish tests, endpoints can be expressed as median lethal loading rate (LL_{50}) when lethal effects occur to 50% of the test population. In cases where no lethal effects are observed at all loadings tested, the result may be expressed as: LL_0 = the highest loading tested. In both cases, results can be expressed in mg/L. For invertebrate and alga tests, endpoints are expressed as median effective loading rate (EL_{50}) or EL_0 in mg/L as discussed above.

Loading rates allow complex, poorly water-soluble substances such as the arylpolyolefins to be compared to more readily soluble substances and pure chemicals on an equal basis. To allow comparison, the toxicity value is expressed as the amount of test material added per unit volume of water when preparing the WAF or WSF.

If test material exposure levels are analytically measured in the test, the endpoints can also be expressed as median lethal concentration (LC_{50}) or median effective

[7] Organization for Economic Cooperation and Development (OECD) (2000). Guidance Document on Aquatic Toxicity Testing of Difficult Substances and Mixtures. OECD Environmental Health and Safety Publications, Series on Testing and Assessment No.23, Paris, France.

concentration (EC_{50}) in mg/L. When working with complex, poorly water-soluble substances, LC/EC_{50} values are often not determined because it can be very difficult to accurately measure test substance exposure levels below 1.0 mg/L.

4.2.2 Aquatic Toxicity of the Arylpolyolefin Category

In general, the toxicity of a substance to an organism is limited by mechanisms of uptake and movement to target organs. Characteristics such as relative smaller molecular weight and a lesser degree of ionization increase the ability of a substance to passively cross biological membranes and exert effects. However, the water-soluble fraction of a compound represents the fraction to which aquatic organisms in the water column will be exposed and the fraction that is available to cause toxicity. Therefore, aquatic toxicity can be either limited by the water solubility of a substance or not determinable, if that substance has very low solubility.

Modeling data suggest that arylpolyolefins have low water solubility. The low water solubility suggests that the aquatic toxicity of these substances will be limited due to low bioavailability to aquatic organisms. As discussed in Section 2.2.7, water solubility testing will be conducted with one of the arylpolyolefin category substances to ensure that the water solubility of the category has been adequately assessed. Aquatic toxicity testing will be conducted on the substance as marketed.

4.2.2.1 Summary of Available Data

There are no aquatic toxicity data available for the members of the arylpolyolefin category.

4.2.2.2 Data Assessment and Test Plan for Acute Aquatic Ecotoxicity

The C_{14}-C_{24} alkaryl derivative (CAS # 115733-08-9) will be evaluated for acute toxicity to a freshwater fish, invertebrate and alga. The C_{14}-C_{24} alkaryl derivative (CAS # 115733-08-9) will be tested because of its lower molecular weight and subsequently higher anticipated water solubility. The data developed for this substance will be used to estimate the aquatic toxicity of the polypropene derivative (CAS # 68081-77-6).

4.3 MAMMALIAN TOXICOLOGY DATA

4.3.1 Physicochemical Properties Relevant to Mammalian Toxicity

Physicochemical properties of chemicals are useful for predicting the routes by which exposure may occur, and in some cases, the mechanism and extent of toxicological responses. The physicochemical properties of the arylpolyolefins are presented in Table

3. These substances are relatively high molecular weight liquids with high octanol/water partition coefficients, low water solubilities and low vapor pressure.

There is little structural diversity in the arylpolyolefin category (Table 2). The arylpolyolefins are characterized by both polypropenyl (branched alkyl side chains) and linear alkyl side chain species. For health-related endpoints, the length or extent of branching of the alkyl side chain is not expected to influence the index of toxicity.

4.3.2 Acute Mammalian Toxicity of the Arylpolyolefin Category

4.3.2.1 Acute Toxicity Test Methodology

Acute toxicity studies investigate the effect(s) of a single exposure to a relatively high dose of a substance. Potential routes of exposure for acute toxicity assays include oral, dermal and inhalation. Oral toxicity assays are conducted by administering test material to fasted animals (typically rats or mice) as a single gavage dose. Acute dermal toxicity tests are conducted by administering test material to the shaved skin on the back of the test animal (typically rats or rabbits) and allowing the test material to stay in contact with the skin application site for a specific duration (usually 24 hours). Acute inhalation toxicity assays are conducted by exposing test animals (typically rats) in a controlled atmosphere to a fixed air concentration of the test substance for a specific duration (typically 4 hours). The test material is generated as a vapor or intentionally aerosolized into respirable particles, then metered into the exposure air at the desired concentration. Preferably, inhalation toxicity studies are conducted using either nose-only or head-only exposure to minimize potential confounding effects resulting from whole-body exposure. Whole body exposure may lead to over-prediction of inhalation toxicity hazard by increasing the body-burden of the test material through skin absorption or ingestion of test material as a consequence of grooming both during and after the inhalation exposure period.

Historically, lethality is a primary end-point of concern in acute toxicity studies, and the traditional index of oral and dermal potency is the median lethal dose that causes mortality in 50 percent of the test animals (LD_{50}). In acute inhalation studies, the traditional measurement of potency is the median lethal concentration of the test material in air that causes mortality in 50 percent of the test animals (LC_{50}). In addition to lethality, acute toxicity studies also provide insights regarding potential systemic toxicity through careful observation and recording of clinical signs and symptoms of toxicity as well as through detailed examination of tissues and organ systems.

Typically, acute oral and dermal toxicity studies are conducted using a limit dose of 5 and 2 g/kg body weight, respectively, and acute inhalation toxicity studies are conducted using a limit dose of 5 mg/L for 4 hours (according to OECD and EPA testing guidelines). Prior to 1990, some acute dermal toxicity studies may have used a limit dose of 5 g/kg. Recently, harmonized EPA testing guidelines (August

1998) have set the limit dose for both oral and dermal acute toxicity studies at 2 g/kg body weight, while the recommended limit concentration for acute inhalation studies has been set at 2 mg/L for 4 hours. The limit dose test method minimizes the number of animals tested by exposing a single group of animals to a large dose (the limit dose) of the test substance. A test substance that shows little or no effects at the limit dose is considered essentially nontoxic, and no further testing is needed. If compound-related mortality is observed at the limit dose, then further testing may be necessary.

4.3.2.2 Summary of Available Data

Acute toxicity data for the arylpolyolefin category is summarized in Table 7. Both category members have been tested for acute oral and acute dermal toxicity. A low order of toxicity was observed for both category members.

4.3.2.2.1 Acute Oral Toxicity

Both of the substances in the arylpolyolefin category have been adequately tested for acute oral toxicity in rats. For both of the substances in the arylpolyolefin category, no mortality was observed for the test material when administered at the limit dose of 5 g/kg. The acute oral LD_{50}s for these substances were greater than the 5 g/kg limit dose, indicating a relatively low order of toxicity.

4.3.2.2.2 Acute Dermal Toxicity

Both of the substances in the arylpolyolefin category have been adequately tested for acute dermal toxicity. For both of the substances in the arylpolyolefin category, no mortality was observed for the test material when administered to rabbits at the limit dose of 2 g/kg. The acute dermal LD_{50}s for these substances were greater than the 2 g/kg limit dose, indicating a relatively low order of toxicity.

4.3.2.3 Data Assessment and Test Plan for Acute Mammalian Toxicity

In total, four adequate acute toxicity studies have been conducted for the arylpolyolefin category members. These studies involved two species of laboratory animals (rats and rabbits); two routes of exposure (oral and dermal); and evaluated the toxicity of both members of the arylpolyolefin category. The data consistently demonstrate a low order of acute toxicity. The low order of toxicity observed for each of the substances in this group is consistent with their similar chemical structure. Therefore, the toxicity of the arylpolyolefin category has been evaluated adequately with respect to acute toxicity endpoints, and no additional acute toxicity testing is proposed.

4.3.3 Genotoxicity of the Arylpolyolefin Category

4.3.3.1 Genotoxicity Test Methodology

Genetic toxicology is concerned with the effects of substances on genetic material (i.e., DNA and chromosomes). Within genetic material, the gene is the simplest functional unit composed of DNA. Mutations are generally non-lethal, heritable changes to genes that may arise spontaneously or as a consequence of xenobiotic exposure. The propensity of a chemical to cause genetic mutations is commonly measured in bacterial and mammalian cells. The simplest test systems measure the occurrence of a base-pair substitution mutation in which a single nucleotide is changed followed by a subsequent change in the complementary nucleotide on the other DNA strand. Frame shift mutations occur following the deletion or insertion of one or more nucleotides, which then changes the "reading frame" for the remainder of the gene or multiple genes. Genetic testing for these types of point mutations is generally accomplished by *in vitro* cellular assays for forward or reverse mutations. A forward mutation occurs when there is a detectable change in native DNA whereas a reverse mutation occurs when a mutated cell is returned to its initial phenotype. Both base-pair substitutions and frame shift mutations are routinely measured in bacterial cells by measuring the ability of a cell to acquire the capability to grow in an environment missing an essential amino acid. In these tests, a large number of cells are examined to demonstrate a significant increase in the frequencies of mutations that occur over the frequency of spontaneous mutations.

Chromosomal aberrations are large-scale numerical or structural alterations in eukaryotic chromosomes including deletions (visualized as breaks), translocations (exchanges), non-disjunction (aneuploidy) and mitotic recombination. Chromosomal breakage is the classical end point in chromosomal aberration assays. Substances that induce structural changes in chromosomes, especially chromosome breaks, are referred to as "clastogens." To visualize chromosomes and chromosomal aberrations following *in vitro* or *in vivo* treatment with a substance, cells are arrested in metaphase, treated to swell the chromosomes, fixed, transferred to slides and stained. The first metaphase following treatment is the time at which the greatest number of cells with damaged chromosomes may be observed. The most frequently used test systems investigate changes in mammalian cells (such as Chinese hamster ovary or lung cells; human or rat lymphocytes; or human, rat or mouse bone marrow cells) following either *in vitro* or *in vivo* exposure to the test substance. The micronucleus test is a common *in vivo* assay that measures the frequency of micronuclei formation (i.e., chromosomal fragments) in polychromatic erythrocytes.

4.3.3.2 Summary of Genotoxicity Data

A summary of the genotoxicity information for the arylpolyolefin category is presented in Table 8. An *in vitro* bacterial gene mutation assays has been conducted for the C_{14}-C_{24} alkaryl derivative (CAS # 115733-08-9). No

chromosomal aberration assays are available for the members of the arylpolyolefin category.

4.3.3.2.1 Bacterial Gene Mutation Assays

The C_{14}-C_{24} alkaryl derivative (CAS # 115733-08-9) has been tested using an *in vitro* bacterial gene mutation assay. The C_{14}-C_{24} alkaryl derivative (CAS # 115733-08-9) did not demonstrate mutagenic activity in the presence or absence of metabolic activation. This test will be used for bridging to the polypropene derivative (CAS # 68081-77-6).

4.3.3.2.2 Chromosomal Aberrations Assays

There are no chromosomal aberration assays available for the members of the arylpolyolefin category.

4.3.3.3 Data Assessment and Test Plan for Genotoxicity

No additional bacterial gene mutation assays are proposed for the arylpolyolefin category. The *in vitro* bacterial gene mutation data for the C_{14}-C_{24} alkaryl derivative (CAS # 115733-08-9) will be bridged to the polypropene derivative (CAS # 68081-77-6). The C_{14}-C_{24} alkaryl derivative (CAS # 115733-08-9) will be tested in an *in vitro* chromosomal aberration assay and the data will be bridged to the polypropene derivative (CAS # 68081-77-6).

4.3.4 Repeated-Dose Toxicity of the Arylpolyolefin Category

4.3.4.1 Repeated-Dose Toxicity Test Methodology

Repeated-dose toxicity studies evaluate the systemic effects of repeated exposure to a chemical over a significant period of the life span of an animal (rats, rabbits, or mice). Chronic repeated-dose toxicity studies are concerned with potential adverse effects upon exposure over the greater part of an organism's life span (e.g., one to two years in rodents). Subchronic repeated-dose studies are also concerned with effects caused by exposure for an extended period, but not one that constitutes a significant portion of the expected life span. Subchronic studies are useful in identifying target organ(s), and they can be used in selecting dose levels for longer-term studies. Typically, the exposure regimen in a subchronic study involves daily exposure (at least 5 consecutive days per week) for a period of at least 28 days or up to 90 days (i.e., 4 to 13 weeks). A recovery period of two to four weeks (generally included in most study designs) following completion of the exposure period provides information on whether or not the effects observed are reversible upon cessation of treatment. The dose levels evaluated in repeated-dose toxicity studies are notably lower than the relatively high limit doses used in acute toxicity studies. The NOAEL (no observed adverse effect level), usually expressed in mg/kg/day, is defined as the dose of test material that produces no significant toxicological effects. In some instances, the test material produces toxicity even at the lowest dose tested (i.e., there is no defined NOAEL); in these cases, the lowest dose that produced an adverse effect is defined as the LOAEL

(lowest observed adverse effect level). Alternatively, results may be reported as the NOEL (no observed effect level) or the LOEL (lowest observed effect level) which are defined, respectively, as the highest dose of the test material that produced no treatment-related effects and the lowest dose that produced treatment-related effects. While these studies are designed to assess systemic toxicity, the study protocol can be modified to incorporate evaluation of potential reproductive and/or developmental effects.

Reproductive and developmental toxicity studies generate information on the effects of a test substance on male and female reproductive performance such as gonadal function, mating behavior, conception, development of the conceptus, parturition and post-partum development of the offspring. Various study designs exist, but they all involve exposure of both male and female animals to the test substance before mating. The rat is most often selected as the test species. The test substance is administered to males and females continuously at several graduated doses for at least two weeks prior to mating and until the animals are sacrificed. The males are treated for at least two more weeks. Male gonadal histopathology is assessed at the end of the study. The females are treated through parturition and early lactation. The adult females and offspring are typically studied until termination on post-natal day 21, or sometimes earlier. In addition to providing data on fertility and reproduction, this study design provides information on potential developmental toxicity following prenatal and limited post-natal exposure to the test substance. A NOAEL or LOAEL is also used to describe the results of these tests, with the exception that these values are derived from effects specific to reproduction or development.

4.3.4.2 Summary of Available Data

There are no repeated-dose or reproductive/developmental toxicity studies available for the members of the arylpolyolefin category.

4.3.4.3 Data Assessment and Test Plan for Repeated-Dose Toxicity

4.3.4.3.1 Repeated-Dose Toxicity

There are no repeated-dose toxicity studies available for the members of the arylpolyolefin category. An oral repeated-dose toxicity study will be conducted on the C_{14}-C_{24} alkaryl derivative (CAS # 115733-08-9) and the data will be bridged to the polypropene derivative (CAS # 68081-77-6).

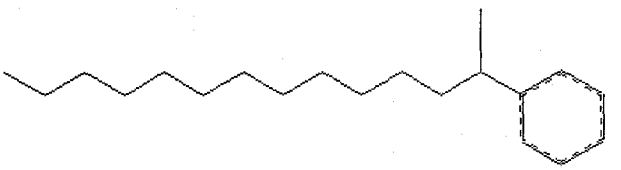
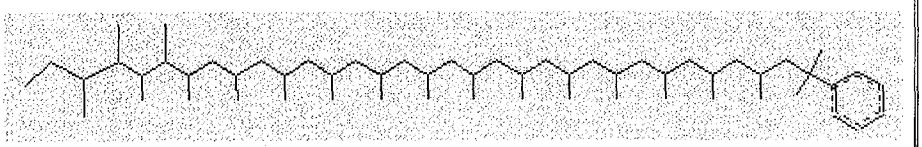
4.3.4.3.2 Reproductive/Developmental Toxicity

There are no reproductive or developmental toxicity studies available for the members of the arylpolyolefin category. A reproductive/developmental toxicity study will be conducted on the C_{14}-C_{24} alkaryl derivative (CAS # 115733-08-9) and the data will be bridged to the polypropene derivative (CAS # 68081-77-6).

Table 1. Registration Numbers and Chemical Names for Arylpolyolefin Category Members

CAS Number	EINECS Number	Chemical Name	Simplified Chemical Name
115733-08-9	None	Benzene, C_{14}-C_{24}-branched and linear alkyl derivatives	C_{14}-C_{24} alkaryl derivative
68081-77-6	None	Benzene, polypropene derivatives	Polypropene derivative

Table 2. Chemical Structures and Names of Arylpolyolefin Category Members

CAS Number	Idealized Chemical Structure and Name
115733-08-9	 C_{14}-C_{24} alkaryl derivative [a]
68081-77-6	 Polypropene derivative [b]

[a] Structure represents the benzene C_{14} alkyl derivative.
[b] Structure represents an intermediate molecular weight range benzene polypropene (C_{52}) derivative.

Table 3. Selected Physicochemical Properties of Arylpolyolefin Category Members and Proposed Testing

CAS Number	Molecular Weight Range[1]	Specific Gravity (@ 15.6°C)	Viscosity (cSt @ 40°C)	Melting Range (°C)	Boiling Range[2] (°C)	Vapor Pressure Range[2] (Pa @ 25°C)	Water Solubility Range[2] (mg/L @ 25°C)	Log Kow Range[2]
115733-08-9	275-415	0.85	21	N.A.	342-458	$1.3e^{-2}$ - $1.7e^{-6}$	$2.0e^{-4}$ - $4.4e^{-9}$ Test	8.9 - 13.8
68081-77-6	387-1228	0.87	93	N.A.	≥388	$\leq 6.2e^{-4}$	$\leq 1.2^{-7}$	≥12.3

[1] Based on molecular weight range of component molecules.
[2] Modeled data based on molecular weight range.
N.A. - Not applicable for liquids at ambient temperatures.

Table 4. Biodegradation, Hydrolysis and Photodegradation Data for Arylpolyolefin Category Members and Proposed Testing

CAS Number	BIODEGRADABILITY	HYDROLYSIS[1]	PHOTODEGRADATION[2]
	Available Data & Proposed Testing	**Available Data & Proposed Testing**	**Available Data & Proposed Modeling**
115733-08-9	**Test**	No testing proposed Arylpolyolefins are not subject to hydrolytic reactions	Direct Photodegradation: No testing needed - Arylpolyolefins are not subject to photolytic reactions Indirect Photodegradation: No testing needed Calculated OH^- Rate Constant (cm^3/molec-sec) = 23e-12 to 37e-12 Calculated Half-life in Air (hrs) = 5.67 to 3.49
68081-77-6	No testing proposed – Bridging	No testing proposed Arylpolyolefins are not subject to hydrolytic reactions	Direct Photodegradation: No testing needed - Arylpolyolefins are not subject to photolytic reactions Indirect Photodegradation: No testing needed Calculated OH^- Rate Constant (cm^3/molec-sec) = ≥31e-12 Calculated Half-life in Air (hrs) = ≤4.10

[1] Chemical components of arylpolyolefin products do not contain functional groups that are subject to hydrolytic reactions; these substances are expected to be stable in water and no testing is necessary.

[2] Chemical components of arylpolyolefin products do not absorb sufficient light energy to result in a structural transformation, therefore these substances are expected to be stable in solution and no testing is necessary; AOPWIN, a subroutine in EPIWIN, was used to model potential indirect photodegradation rates for selected chemical structures that represent arylpolyolefin category members (see Section 4.1.4.1).

Table 5. Distribution and Fugacity Data for Selected Chemical Components of Arylpolyolefin Category Members

CAS Number	PERCENT DISTRIBUTION AND FUGACITY[1]						
	Available Modeling Data						
	Air (%)	Water (%)	Soil (%)	Sediment (%)	Suspended Sediment (%)	Biota (%)	Fugacity (uPa)
115733-08-9 Benzene C_{14} alkyl derivative[a]	0.102	1.3e-4	97.7	2.170	0.068	0.005	9.18e-3
115733-08-9 Benzene C_{24} alkyl derivative[a]	0.026	1.8e-9	97.7	2.172	0.068	0.006	1.54e-3
68081-77-6 Benzene C_{22} polypropene[a]	0.027	5.5e-8	97.7	2.172	0.068	0.006	1.71e-3

[1] The EQC Level I model as referenced in Mackay et al., 1996 (Environ. Toxicol. Chem. 15:1627-1637), was used to calculate environmental partitioning data for selected chemical structures that represent arylpolyolefins (see Section 4.1.5.1).

[a] The structure used for modeling.

Table 6. Aquatic Toxicity Data for Arylpolyolefin Category Members and Proposed Testing

CAS Number	FISH ACUTE TOXICITY 96-hr LC_{50} (mg/L)	INVERTEBRATE ACUTE TOXICITY 48-hr EC_{50} (mg/L)	ALGA TOXICITY 96-hr EC_{50} (mg/L)
	Available Data & Proposed Testing	**Available Data & Proposed Testing**	**Available Data & Proposed Testing**
115733-08-9	**Test**	**Test**	**Test**
68081-77-6	No testing proposed – Bridging	No testing proposed – Bridging	No testing proposed – Bridging

Table 7. Evaluation of Acute Mammalian Toxicity of Arylpolyolefin Category Members

CAS Number	ACUTE ORAL TOXICITY[1] Available Data	ACUTE DERMAL TOXICITY[1] Available Data
115733-08-9	LD_{50} > 5 g/kg (rat)	LD_{50} > 2 g/kg (rabbit)
68081-77-6	LD_{50} > 5 g/kg (rat)	LD_{50} > 2 g/kg (rabbit)

[1] Toxicity endpoints are expressed as median lethal dose (LD_{50}) for acute oral and dermal toxicity. The LD_{50} is defined as the dose that is lethal to 50% of the test organisms. The greater the LD_{50}, the lower the toxicity.

Table 8. Evaluation of Genotoxicity of Arylpolyolefin Category Members and Proposed Testing

CAS Number	GENE MUTATION ASSAY	CHROMOSOMAL ABERRATION ASSAY
	Available Data & Proposed Testing	**Available Data & Proposed Testing**
115733-08-9	*In vitro* Bacterial Reverse Mutation Assay – With and Without S-9 – Not Mutagenic	**Test**
68081-77-6	No testing proposed – Bridging	No testing proposed– Bridging

Table 9. Evaluation of Repeated-Dose Mammalian Toxicity of Arylpolyolefin Category Members and Proposed Testing

CAS Number	REPEATED-DOSE TOXICITY Available Data & Proposed Testing	REPRODUCTIVE/DEVELOPMENTAL TOXICITY Available Data & Proposed Testing
115733-08-9	**Test**	**Test**
68081-77-6	No testing proposed – Bridging	No testing proposed – Bridging

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Table 10. Summary of Data for Arylpolyolefin Category Members and Proposed Testing

CAS Number	Environmental Fate					Ecotoxicity			Human Health Effects				
	Physical Chem	Photodeg	Hydrolysis	Fugacity	Biodeg	Acute Fish Toxicity	Acute Invert Toxicity	Algal Toxicity	Acute Toxicity	Point Mutations	Chrom Effects	Sub-chronic	Repro/ Develop
115733-08-9	C / T	D / C	D	C	T	T	T	T	A	A	T	T	T
68081-77-6	C / B	D / C	D	C	B	B	B	B	A	B	B	B	B

A Adequate data available
B Bridging
C Computer modeling completed
D Technical discussion completed
T Test

AR201-14132B

Substance Group:	**Group 2**
Summary Prepared by:	**Petroleum Additives Panel** **Health & Environmental Research Task Group**
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1.0 Physicochemical Properties

Robust Summary #: 2-Physchem-1 (Boiling Point-Range)

Test Substance*:	Other TS
Method/Guideline:	Calculated values using MPBPWIN version 1.40, a subroutine of the computer program EPIWIN version 3.04
Year (guideline):	1999
Type (test type):	Not applicable
GLP:	Not applicable
Year (study performed):	Not applicable
Estimation Pressure:	760 mm Hg
Test Conditions: • **Note: Concentration prep., vessel type, replication, test conditions.**	Boiling point calculated by MPBPWIN subroutine, which is based on the method of S. Stein and R. Brown in "Estimation of Normal Boiling Points from Group Contributions". 1994. J. Chem. Inf. Comput. Sci. 34: 581-587.
Results: **Units/Value:** • **Note: Deviations from protocol or guideline, analytical method.**	Substance Component — Calculated BP (°C) CAS# 115733-08-9 Benzene, C_{14} alkyl derivative 342 Benzene, C_{24} alkyl derivative 458 CAS# 68081-77-6 Benzene, C_{22} polypropene 388 Commercial substances in this category have a carbon number distribution between C20 and C30 or C28 and C88. The three chemicals selected to represent the atmospheric oxidation potential range of this category include a C20, C30, and C28 arylpolyolefin that have common structures. The modeling data for physicochemical endpoints in Sections 2.2.5 to 2.2.7 are presented as ranges for category members, where possible, and are based on the highest and lowest molecular weight derivative in each member. For example, structures representing the C_{14}-C_{24} alkaryl derivative (CAS # 115733-08-9) include a benzene C_{14} alkyl derivative and a benzene C_{24} alkyl derivative. Whereas, structures representing the polypropene

	derivative (CAS # 68081-77-6) include only the benzene C_{22} polypropene lowest molecular weight derivative; the benzene C_{82} polypropene highest molecular weight derivative has not been modeled as the molecular weight of this derivative falls outside of the applicable range of the EPIWIN modeling program.
Test Substance:	• CAS# 115733-08-9; Benzene C_{14}-C_{24} branched and linear alkyl derivatives • CAS# 68081-77-6; Benzene polypropene derivatives Arylpolyolefins are manufactured by mixing anhydrous alkylate (linear or branched) with benzene in the presence of catalyst and heat. More information on the Arylpolyolefin Category can be found in the American Chemistry Council; Petroleum Additives Panel; Health, Environmental, Regulatory, Task Group, High Production Volume test plan for this category (1). 1. Health, Environmental, Regulatory, Task Group (HERTG). 2002. High Production Volume (HPV) Chemical Challenge Program Test Plan For The Arylpolyolefin Category. American Chemistry Council, Petroleum Additives Panel, HERTG.
Conclusion:	Modeling data indicate that the boiling range of category members can range from 342 to 458°C for the C_{14}-C_{24} alkaryl derivative (CAS # 115733-08-9) and can be >388°C for the polypropene derivative (CAS # 68081-77-6).
Reliability:	(2) Reliable with restrictions The results include calculated values based on chemical structure and represent a potential boiling range for substances with the 2 CAS numbers listed under test substance.
Reference:	Boiling point calculated by MPBPWIN subroutine, which is contained in the computer program: EPIWIN. 1999. Estimation Program Interface for Windows, version 3.04. Syracuse Research Corporation, Syracuse, NY, USA.
Other (source):	American Chemistry Council; Petroleum Additives Panel; Health, Environmental, Regulatory, Task Group

* Other TS is an option in the "test substance" pick list within the IUCLID data entry field for "melting point". Selecting this option refers the reader to information in the "freetext" field for "test substance".

Robust Summary #: 2-Physchem-2 (Vapor Pressure Range)

Test Substance*:	Other TS
Method/Guideline:	Calculated values using MPBPWIN version 1.40, a subroutine of the computer program EPIWIN version 3.04
Year (guideline):	1999
Type (test type):	Not applicable
GLP:	Not applicable
Year (study performed):	Not applicable
Estimation Temperature:	25°C
Test Conditions: • **Note: Concentration prep., vessel type, replication, test conditions.**	Vapor Pressure calculated by MPBPWIN subroutine, which is based on the average result of the methods of Antoine and Grain. Both methods use boiling point for the calculation. The Antoine method is described in: Handbook of Chemical Property Estimation. Chapter 14. W.J. Lyman, W.F. Reehl and D.H. Rosenblatt, Eds. Washington, D.C.: American Chemical Society. 1990. The modified Grain method is described in: Neely and Blau's Environmental Exposure from Chemicals, Volume 1. 1985. CRC Press. Page 31.
Results: **Units/Value:** • **Note: Deviations from protocol or guideline, analytical method.**	Substance Component — Calculated VP (Pa) CAS# 115733-08-9 Benzene, C_{14} alkyl derivative $1.3e^{-2}$ Benzene, C_{24} alkyl derivative $1.7e^{-6}$ CAS# 68081-77-6 Benzene, C_{22} polypropene $6.2e^{-4}$ Commercial substances in this category have a carbon number distribution between C20 and C30 or C28 and C88. The three chemicals selected to represent the atmospheric oxidation potential range of this category include a C20, C30, and C28 arylpolyolefin that have common structures. The modeling data for physicochemical endpoints in Sections 2.2.5 to 2.2.7 are presented as ranges for category members, where possible, and are based on the highest and lowest molecular weight derivative in each member. For

	example, structures representing the C_{14}-C_{24} alkaryl derivative (CAS # 115733-08-9) include a benzene C_{14} alkyl derivative and a benzene C_{24} alkyl derivative. Whereas, structures representing the polypropene derivative (CAS # 68081-77-6) include only the benzene C_{22} polypropene lowest molecular weight derivative; the benzene C_{82} polypropene highest molecular weight derivative has not been modeled as the molecular weight of this derivative falls outside of the applicable range of the EPIWIN modeling program.
Test Substance:	• CAS# 115733-08-9; Benzene C_{14}-C_{24} branched and linear alkyl derivatives • CAS# 68081-77-6; Benzene polypropene derivatives Arylpolyolefins are manufactured by mixing anhydrous alkylate (linear or branched) with benzene in the presence of catalyst and heat. More information on the Arylpolyolefin Category can be found in the American Chemistry Council; Petroleum Additives Panel; Health, Environmental, Regulatory, Task Group, High Production Volume test plan for this category (1). 1. Health, Environmental, Regulatory, Task Group (HERTG). 2002. High Production Volume (HPV) Chemical Challenge Program Test Plan For The Arylpolyolefin Category. American Chemistry Council, Petroleum Additives Panel, HERTG.
Conclusion:	Modeling data indicate that the vapor pressure range of category members can range from $1.3e^{-2}$ to $1.7e^{-6}$ Pa at 25 °C for the C_{14}-C_{24} alkaryl derivative (CAS # 115733-08-9) and can be $<6.2e^{-4}$ Pa at 25 °C for the polypropene derivative (CAS # 68081-77-6).
Reliability:	(2) Reliable with restrictions The results include calculated values based on chemical structure and represent a potential vapor pressure range for substances with the 2 CAS numbers listed under test substance.
Reference:	Melting point calculated by MPBPWIN subroutine, which is contained in the computer program: EPIWIN. 1999. Estimation Program Interface for Windows, version 3.04. Syracuse Research Corporation, Syracuse, NY, USA.

Other (source):	American Chemistry Council; Petroleum Additives Panel; Health, Environmental, Regulatory, Task Group

* Other TS is an option in the "test substance" pick list within the IUCLID data entry field for "melting point". Selecting this option refers the reader to information in the "freetext" field for "test substance".

Robust Summary #: 2-Physchem-3 (Water Solubility Range)

Test Substance*:	Other TS
Method/Guideline:	Calculated values using WSKOWWIN version 1.36, a subroutine of the computer program EPIWIN version 3.04
Year (guideline):	1999
Type (test type):	Not applicable
GLP:	Not applicable
Year (study performed):	Not applicable
Estimation Temperature:	25°C
Test Conditions: • **Note: Concentration prep., vessel type, replication, test conditions.**	Water Solubility calculated by WSKOWWIN subroutine, which is based on a Kow correlation method described by W. Meylan, P. Howard and R. Boethling in "Improved method for estimating water solubility from octanol/water partition coefficient". Environ. Toxicol. Chem. 15:100-106. 1995.
Results: **Units/Value:** • **Note: Deviations from protocol or guideline, analytical method.**	Substance Component — Calculated WS (mg/L) CAS# 115733-08-9 Benzene, C_{14} alkyl derivative $2.0e^{-4}$ Benzene, C_{24} alkyl derivative $4.4e^{-9}$ CAS# 68081-77-6 Benzene, C_{22} polypropene 1.2^{-7} Commercial substances in this category have a carbon number distribution between C20 and C30 or C28 and C88. The three chemicals selected to represent the atmospheric oxidation potential range of this category include a C20, C30, and C28 arylpolyolefin that have common structures. The modeling data for physicochemical endpoints in Sections 2.2.5 to 2.2.7 are presented as ranges for category members, where possible, and are based on the highest and lowest molecular weight derivative in each member. For example, structures representing the C_{14}-C_{24} alkaryl derivative (CAS # 115733-08-9) include a benzene C_{14} alkyl derivative and a benzene C_{24} alkyl derivative. Whereas, structures representing the polypropene derivative (CAS # 68081-77-6) include only the

	benzene C_{22} polypropene lowest molecular weight derivative; the benzene C_{82} polypropene highest molecular weight derivative has not been modeled as the molecular weight of this derivative falls outside of the applicable range of the EPIWIN modeling program.
Test Substance:	• CAS# 115733-08-9; Benzene C_{14}-C_{24} branched and linear alkyl derivatives • CAS# 68081-77-6; Benzene polypropene derivatives Arylpolyolefins are manufactured by mixing anhydrous alkylate (linear or branched) with benzene in the presence of catalyst and heat. More information on the Arylpolyolefin Category can be found in the American Chemistry Council; Petroleum Additives Panel; Health, Environmental, Regulatory, Task Group, High Production Volume test plan for this category (1). 1. Health, Environmental, Regulatory, Task Group (HERTG). 2002. High Production Volume (HPV) Chemical Challenge Program Test Plan For The Arylpolyolefin Category. American Chemistry Council, Petroleum Additives Panel, HERTG.
Conclusion:	Modeling data indicate that the water solubility range of category members can range from $2.0e^{-4}$ to $4.4e^{-9}$ mg/L at 25 °C for the C_{14}-C_{24} alkaryl derivative (CAS # 115733-08-9) and can be $<1.2e^{-7}$ mg/L at 25 °C for the polypropene derivative (CAS # 68081-77-6).
Reliability:	(2) Reliable with restrictions The results include calculated values based on chemical structure and represent a potential water solubility range for substances with the 2 CAS numbers listed under test substance.
Reference:	Water solubility values calculated by WSKOWWIN subroutine, which is contained in the computer program: EPIWIN. 1999. Estimation Program Interface for Windows, version 3.04. Syracuse Research Corporation, Syracuse, NY, USA.
Other (source):	American Chemistry Council; Petroleum Additives Panel; Health, Environmental, Regulatory, Task Group

* Other TS is an option in the "test substance" pick list within the IUCLID data entry field for "melting point". Selecting this option refers the reader to information in the "freetext" field for "test substance".

Robust Summary #: 2-Physchem-4 (Log Kow Range)

Test Substance*:	Other TS
Method/Guideline:	Calculated values using KOWWIN version 1.65, a subroutine of the computer program EPIWIN version 3.04
Year (guideline):	1999
Type (test type):	Not applicable
GLP:	Not applicable
Year (study performed):	Not applicable
Estimation Temperature:	25°C
Test Conditions: • **Note: Concentration prep., vessel type, replication, test conditions.**	Octanol / Water Partition Coefficient estimations calculated by KOWWIN subroutine, which is based on an atom/fragment contribution method of W. Meylan and P. Howard in "Atom/fragment contribution method for estimating octanol-water partition coefficients". 1995. J. Pharm. Sci. 84:83-92.
Results: **Units/Value:** • **Note: Deviations from protocol or guideline, analytical method.**	Substance Component — Calculated Log Kow CAS# 115733-08-9 Benzene, C_{14} alkyl derivative 8.9 Benzene, C_{24} alkyl derivative 13.8 CAS# 68081-77-6 Benzene, C_{22} polypropene 12.3 Commercial substances in this category have a carbon number distribution between C20 and C30 or C28 and C88. The three chemicals selected to represent the atmospheric oxidation potential range of this category include a C20, C30, and C28 arylpolyolefin that have common structures. The modeling data for physicochemical endpoints in Sections 2.2.5 to 2.2.7 are presented as ranges for category members, where possible, and are based on the highest and lowest molecular weight derivative in each member. For example, structures representing the C_{14}-C_{24} alkaryl derivative (CAS # 115733-08-9) include a benzene C_{14} alkyl derivative and a benzene C_{24} alkyl derivative. Whereas, structures representing the polypropene derivative (CAS # 68081-77-6) include only the benzene C_{22} polypropene lowest molecular weight

	derivative; the benzene C_{82} polypropene highest molecular weight derivative has not been modeled as the molecular weight of this derivative falls outside of the applicable range of the EPIWIN modeling program.
Test Substance:	• CAS# 115733-08-9; Benzene C_{14}-C_{24} branched and linear alkyl derivatives • CAS# 68081-77-6; Benzene polypropene derivatives Arylpolyolefins are manufactured by mixing anhydrous alkylate (linear or branched) with benzene in the presence of catalyst and heat. More information on the Arylpolyolefin Category can be found in the American Chemistry Council; Petroleum Additives Panel; Health, Environmental, Regulatory, Task Group, High Production Volume test plan for this category (1). 1. Health, Environmental, Regulatory, Task Group (HERTG). 2002. High Production Volume (HPV) Chemical Challenge Program Test Plan For The Arylpolyolefin Category. American Chemistry Council, Petroleum Additives Panel, HERTG.
Conclusion:	Modeling data indicate that the log of the octanol-water partition coefficients (log K_{ow}) for category members are estimated to be >8.9.
Reliability:	(2) Reliable with restrictions The results include calculated values based on chemical structure and represent a potential log Kow range for substances with the 2 CAS numbers listed under test substance.
Reference:	Log Kow values calculated by KOWWIN subroutine, which is contained in the computer program: EPIWIN. 1999. Estimation Program Interface for Windows, version 3.04. Syracuse Research Corporation, Syracuse, NY, USA.
Other (source):	American Chemistry Council; Petroleum Additives Panel; Health, Environmental, Regulatory, Task Group

* Other TS is an option in the "test substance" pick list within the IUCLID data entry field for "melting point". Selecting this option refers the reader to information in the "freetext" field for "test substance".

2.1 Hydrolysis

Robust Summary #: 2-Hydro-1

Test Substance*:	Other TS
Method/Guideline:	Other: Technical discussion
Year (guideline):	Not applicable
Type (test type):	Not applicable
GLP (Y/N):	Not applicable
Year (study performed):	Not applicable
Analytical Monitoring:	Not applicable
Test Conditions: • **Note: Concentration preparation, vessel type, volume, replication, deviations from guideline or protocol**	Not applicable
Results: **Units/Value:** • **Note: Analytical method, observations, half-lives by pH, degradation products**	Not applicable
Test Substance:	CAS# 115733-08-9; Benzene C_{14}-C_{24} branched and linear alkyl derivatives CAS# 68081-77-6; Benzene polypropene derivatives Arylpolyolefins are manufactured by mixing anhydrous alkylate (linear or branched) with benzene in the presence of catalyst and heat. More information on the Arylpolyolefin category can be found in the American Chemistry Council; Petroleum Additives Panel; Health, Environmental, Regulatory, Task Group, High Production Volume test plan for this category (1). 1. Health, Environmental, Regulatory, Task Group

	(HERTG). 2002. High Production Volume (HPV) Chemical Challenge Program Test Plan For The Arylpolyolefin Category. American Chemistry Council, Petroleum Additives Panel, HERTG.
Conclusion:	**Summary** In the environment, hydrolysis will not contribute to the degradation of chemicals in the Arylpolyolefin Category. Two CAS numbers identify substances in this category: • 115733-08-9; Benzene C_{14}-C_{24} branched and linear alkyl derivatives • 68081-77-6; Benzene polypropene derivatives As discussed below, the chemicals in these streams are composed of carbon and hydrogen and are not amenable to hydrolysis because of their molecular structure and the chemical reaction required for this type of transformation to occur. The Arylpolyolefin Category Commercial arylpolyolefins are manufactured by reacting anhydrous alkylate (linear or branched) with benzene in the presence of catalyst and heat. Linear alkylbenzenes use linear alpha olefins with $AlCl_3$ and HF as the preferred catalyst. Branched alkylbenzenes start with a tetrapropenyl (C_3) stream using HF as the preferred catalyst, but triethyl aluminum ($AlEt_3$) has also been used as a catalyst. Commercial substances in this category have a carbon number distribution between C20 to C30 or C28 to C88. The chemical constituents of these substances are composed of carbon and hydrogen and share a similar structure; they are linear or branched alkyl benzenes with alkyl groups ranging between C14 and C82. Because of their chemical similarity, this group is considered a category for purposes of the High Production Volume (HPV) Chemical Program, and designated Arypolyolefin. **Hydrolysis of Hydrocarbons as a Function of Molecular Structure** Hydrolysis of an organic molecule occurs when a molecule (R-X) reacts with water (H_2O) to form a new carbon-oxygen bond after the carbon-X bond is cleaved (1,2). Mechanistically, this reaction is referred to as a nucleophilic substitution reaction, where X is the leaving group being replaced by the incoming nucleophilic oxygen from the water molecule. The leaving group, X, must be a molecule other than carbon because for hydrolysis to occur, the R-X bond cannot be a carbon-carbon bond.

	The carbon atom lacks sufficient electronegativity to be a good leaving group and carbon-carbon bonds are too stable (high bond energy) to be cleaved by nucleophilic substitution. Thus, hydrocarbons are not subject to hydrolysis (2) and this fate process will not contribute to the degradative loss of chemical components in this category from the environment.
	Under strongly acidic conditions a carbon-carbon double bond can react with water by an addition reaction mechanism (1). The reaction product is an alcohol. This reaction is not considered to be hydrolysis because the carbon-carbon linkage is not cleaved and because the reaction is freely reversible (2). Chemicals that have a potential to hydrolyze include alkyl halides, amides, carbamates, carboxylic acid esters and lactones, epoxides, phosphate esters, and sulfonic acid esters (3). The chemicals in this category are arylpolyolefins that contain double bonds in the aromatic ring. The remaining chemical structure contains saturated hydrocarbons (paraffins). These chemicals contain only carbon and hydrogen. As such, their molecular structure is not subject to the hydrolytic mechanism discussed above. Therefore, chemicals in the Arylpolyolefin Category have a very low potential to hydrolyze, and this degradative process will not contribute to their removal in the environment. <u>References</u> 1. Gould, E.S. 1959. Mechanism and Structure in Organic Chemistry, Holt, Reinhart and Winston, New York, NY, USA. 2. Harris, J.C. 1982. "Rate of Hydrolysis," Chapter 7 in: W.J. Lyman, W.F. Reehl, and D.H. Rosenblatt, eds., Handbook of Chemical Property Estimation Methods, McGraw-Hill Book Company, New York, NY, USA. 3. Neely, W. B. 1985. Hydrolysis. In: W. B. Neely and G. E. Blau, eds. Environmental Exposure from Chemicals. Vol I., pp. 157-173. CRC Press, Boca Raton, FL, USA.
Reliability:	Not applicable
Reference:	American Chemistry Council; Petroleum Additives Panel; Health, Environmental, Regulatory, Task Group. 2002. Hydrolysis: Arylpolyolefin Category. Rosslyn, VA, USA.

Other (source):	American Chemistry Council; Petroleum Additives Panel; Health, Environmental, Regulatory, Task Group

* Other TS is an option in the "test substance" pick list within the IUCLID data entry field for "hydrolysis". Selecting this option refers the reader to information in the "freetext" field for "test substance".

2.2 Photodegradation (Direct & Indirect)

Robust Summary #: 2-Photo-1 (Direct)

Test Substance*:	Other TS
Method/Guideline:	Other: Technical discussion
Year (guideline):	Not applicable
GLP (Y/N):	Not applicable
Year (study performed):	Not applicable
Type (air, soil, water, other):	Water
Test Substance:	CAS# 115733-08-9; Benzene C_{14}-C_{24} branched and linear alkyl derivatives CAS# 68081-77-6; Benzene polypropene derivatives Arylpolyolefins are manufactured by mixing anhydrous alkylate (linear or branched) with benzene in the presence of catalyst and heat. More information on the Arylpolyolefin category can be found in the American Chemistry Council; Petroleum Additives Panel; Health, Environmental, Regulatory, Task Group, High Production Volume test plan for this category (1). 1. Health, Environmental, Regulatory, Task Group (HERTG). 2002. High Production Volume (HPV) Chemical Challenge Program Test Plan For The Arylpolyolefin Category. American Chemistry Council, Petroleum Additives Panel, HERTG.
Light Source:	Not applicable
Light Spectrum: • **Wave length value (upper/lower)**	Not applicable
Relative Intensity:	Not applicable
Test Substance Spectrum:	Not applicable
Test Conditions: • **Note: Concentration, temperature, test system type, replication, deviations from**	Not applicable

guideline or protocol	
Direct Photolysis: • **Results: half-life, % degrad., quantum yield**	Not applicable
Indirect Photolysis: • **Results: type of sensitizer, concentration of sensitizer, rate const., % degrad., half-life**	Not applicable
Degradation Products: • **Note: Identification, concentration**	Not applicable
Conclusion:	**Technical Summary** In the environment, direct photolysis will not contribute to the degradation of constituent chemicals of substances in the Arylpolyolefin Category. Two CAS numbers identify substances in this category: • 115733-08-9; Benzene C_{14}-C_{24} branched and linear alkyl derivatives • 68081-77-6; Benzene polypropene derivatives The direct photolysis of an organic molecule occurs when it absorbs sufficient light energy to result in a structural transformation (1). The reaction process is initiated when light energy in a specific wavelength range elevates a molecule to an electronically excited state. However, the excited state is competitive with various deactivation processes that can result in the return of the molecule to a non excited state. The absorption of light in the ultra violet (UV)-visible range, 110-750 nm, can result in the electronic excitation of an organic molecule. Light in this range contains energy of the same order of magnitude as covalent bond dissociation energies (1). Higher wavelengths (e.g. infrared) result only in vibrational and rotational transitions, which do not tend to produce structural changes to a molecule. The stratospheric ozone layer prevents UV light of less than 290 nm from reaching the earth's surface. Therefore, only light at wavelengths between 290 and 750 nm can result in photochemical transformations in the environment (1).

	Although the absorption of UV light in the 290-750 nm range is necessary, it is not always sufficient for a chemical to undergo photochemical degradation. Energy may be re-emitted from an excited molecule by mechanisms other than chemical transformation, resulting in no change to the parent molecule.
Conclusion: (continued)	A conservative approach to estimating a potential photochemical degradation rate is to assume that degradation will occur in proportion to the amount of light wavelengths >290 nm absorbed by the molecule (2). Saturated hydrocarbons do not absorb light above 200 nm. Therefore, those constituents of substances in this category will not exhibit photolytic degradation. Single ring aromatics do not absorb sufficient light energy above 290 nm to cause photolysis (1). Therefore, the arylpolyolefins in this category are also not subject to photolytic processes. References 1. Harris, J. C. 1982. "Rate of Aqueous Photolysis," Chapter 8 in: W. J. Lyman, W. F. Reehl, and D. H. Rosenblatt, eds., Handbook of Chemical Property Estimation Methods, McGraw-Hill Book Company, New York, USA. 2. Zepp, R. G. and D. M. Cline. 1977. Rates of Direct Photolysis in the Aqueous Environment, Environ. Sci. Technol., 11:359-366.
Reliability:	Not applicable
Reference:	American Chemistry Council; Petroleum Additives Panel; Health, Environmental, Regulatory, Task Group. 2002. Hydrolysis: Arylpolyolefin Category. Rosslyn, VA, USA.
Other (source):	American Chemistry Council; Petroleum Additives Panel; Health, Environmental, Regulatory, Task Group

* Other TS is an option in the Test Substance pick list within the IUCLID data entry field for Photodegradation (direct). Selecting this option refers the reader to information in the "freetext" field for "test substance".

Robust Summary #: 2-Photo-2 (Indirect)

Test Substance*:	Other TS
Method/Guideline:	Calculated values using AOPWIN version 1.89, a subroutine of the computer program EPIWIN version 3.04
Year (guideline):	1999
GLP (Y/N):	Not applicable
Year (study performed):	Not applicable
Type (air, soil, water, other):	Not applicable
Light Source:	Sunlight
Light Spectrum: • **Wave length value (upper/lower)**	Natural sunlight
Relative Intensity:	1
Test Substance Spectrum:	Not applicable
Test Conditions: • **Note: Concentration, temperature, test system type, replication, deviations from guideline or protocol**	Indirect photodegradation, or atmospheric oxidation potential, is based on the structure-activity relationship methods developed by R. Atkinson. Temperature: 25°C Sensitizer: OH radical Concentration of Sensitizer: 1.5 E^6 OH radicals/cm^3
Direct Photolysis: • **Results: half-life, % degradation, quantum yield**	Not applicable
Indirect Photolysis: • **Results: type of sensitizer, concentration of sensitizer, rate constant, % degradation, half-life**	AOPWIN estimates the rate constant for the atmospheric, gas-phase reaction between photochemically produced hydroxyl radicals and organic chemicals. The rate constants estimated by the program are then used to calculate atmospheric half-lives for organic compounds based upon average atmospheric concentrations of hydroxyl radicals. Since the reactions only take place in the presence of sunlight, the atmospheric half-life is normalized for a 12-hour day.

	Calculated* OH- Rate Constant Substance Component half-life (hrs) (cm^3/molecule-sec) CAS# 115733-08-9 Benzene, C_{14} alkyl derivative 5.67 23e-12 Benzene, C_{24} alkyl derivative 3.49 37e-12 CAS# 68081-77-6 Benzene, C_{22} polypropene 4.10 31e-12 * Atmospheric half-life values are based on a 12-hr day. Commercial substances in this category have a carbon number distribution between C20 and C30 or C28 and C88. The three chemicals selected to represent the atmospheric oxidation potential range of this category include a C20, C30, and C28 arylpolyolefin that have common structures. Calculated air oxidation potential values are presented as ranges for category members, where possible, and are based on the highest and lowest molecular weight derivative in each member. For example, structures representing the C_{14}-C_{24} alkaryl derivative (CAS # 115733-08-9) include a benzene C_{14} alkyl derivative and a benzene C_{24} alkyl derivative. Whereas, structures representing the polypropene derivative (CAS # 68081-77-6) include only the benzene C_{22} polypropene lowest molecular weight derivative; the benzene C_{82} polypropene highest molecular weight derivative has not been modeled as the molecular weight of this derivative falls outside of the applicable range of the EPIWIN modeling program. References 1. Atkinson, R. 1988. Estimation of gas-phase hydroxyl radical rate constants for organic chemicals. Environ. Toxicol. Chem. **7**:435-442. 2. Atkinson, R. 1989. Kinetics and mechanisms of the gas-phase reactions of the hydroxyl radical with organic compounds. J. Phys. Chem. Ref. Data Monograph No. 1, Amer. Inst. Physics & Amer. Chem. Soc., New York, NY, USA. 3. Meylan, W.M. and P.H. Howard. 1993. Computer estimation of the atmospheric gas-phase reaction rate of organic compounds with hydroxyl radicals

	and ozone. Chemosphere. **12**:2293-2299.
Degradation Products: • **Note: Identification, concentration**	Unknown
Test Substance:	• CAS# 115733-08-9; Benzene C_{14}-C_{24} branched and linear alkyl derivatives • CAS# 68081-77-6; Benzene polypropene derivatives Arylpolyolefins are manufactured by mixing anhydrous alkylate (linear or branched) with benzene in the presence of catalyst and heat. More information on the Arylpolyolefin Category can be found in the American Chemistry Council; Petroleum Additives Panel; Health, Environmental, Regulatory, Task Group, High Production Volume test plan for this category (4). 4. Health, Environmental, Regulatory, Task Group (HERTG). 2002. High Production Volume (HPV) Chemical Challenge Program Test Plan For The Arylpolyolefin Category. American Chemistry Council, Petroleum Additives Panel, HERTG.
Conclusion:	Atmospheric oxidation can contribute to the degradation of substances in this category. However, their low vapor pressures suggest that constituents of these substances will not partition to a great extent into the air phase where this reaction takes place. Therefore, this degradation process is not expected to significantly contribute to the degradative loss of these substances in the environment. Based on calculated values, substances in this category can have an atmospheric half-life range of 3.5 to 5.7 hours. These data suggest that the fraction of constituents that do partition to the air phase will degrade rapidly. These data represent a key study for characterizing the atmospheric oxidation potential of the Arylpolyolefin Category, which includes benzene C_{14}-C_{24} alkyl derivatives (CAS # 115733-08-9) and benzene polypropene derivatives (CAS # 68081-77-6).
Reliability:	(2) Reliable with restrictions The results include values calculated using the AOPWIN program and represent a potential atmospheric half-life range for substances with the 2 CAS numbers listed under test substance.
Reference:	Meylan, M., SRC. 1994-1999. AOPWIN is contained in the computer program EPIWIN. 1999. Estimation

	Program Interface for Windows, version 3.04. Syracuse Research Corporation, Syracuse, NY, USA.
Other (source):	American Chemistry Council; Petroleum Additives Panel; Health, Environmental, Regulatory, Task Group

* Other TS is an option in the "test substance" pick list within the IUCLID data entry field for "photodegradation". Selecting this option refers the reader to information in the "freetext" field for "test substance".

Robust Summary #: 2-Fugacity-1

Test Substance*:	Other TS
Method/Guideline:	Calculated according to Mackay Level I, EQC Model version 1.01
Year (guideline):	1997
Type (test type):	Not applicable
GLP:	Not applicable
Year (study performed):	Not applicable
Estimation Temperature:	25°C
Test Conditions: • **Note: Concentration prep., vessel type, replication, test conditions.**	The EQC Level I is a steady state, equilibrium model that utilizes the input of basic chemical properties including molecular weight, vapor pressure, and water solubility to calculate distribution within a standardized regional environment. Physical properties used with the model were calculated by the EPIWIN Estimation v 3.04 program (1). Output data from the equilibrium model provide basic information on the potential distribution of chemicals between selected environmental compartments (i.e., air, water, soil, sediment, suspended sediment, biota). 1. EPIWIN. 1999. Estimation Program Interface for Windows, version 3.04. Syracuse Research Corporation, Syracuse, NY, USA.
Results: **Units/Value:** • **Note: Deviations from protocol or guideline, analytical method.**	The following chemicals are representative of the two CAS numbers in the Arylpolyolefin Category, each of which contains complex, multi-constituent substances. The partitioning data characterize the range of constituent chemicals in each substance as well as the overall partitioning behavior of these substances. Calculated* Percent Distribution Substance Component — Soil — Sediment CAS# 115733-08-9 Benzene, C_{14} alkyl derivative — 97.7 — 2.17 Benzene, C_{24} alkyl derivative — 97.7 — 2.17

	CAS# 68081-77-6 Benzene, C_{22} polypropene97.7 2.17 Benzene, C_{82} polypropene97.8 2.17 * Distribution values determined using input data calculated by the EPIWIN program.
Results: (continued) **Units/Value:** **Note: Deviations from protocol or guideline, analytical method.**	Distribution of representative chemicals to each remaining compartment (air, water, suspended sediment, biota) was calculated as less than 0.2%. Potential for mobility throughout the environment is expected to be low due to the relatively high log Kow values and low water solubility of constituent chemicals. Commercial substances in this category have a carbon number distribution between either C20 and C30 or C28 and C88. The four chemicals selected to represent the transport / distribution range of this category include a C20, C30, C28, and C88 arylpolyolefin that have common structures and represent the potential range of data for the two category substances.
Test Substance:	• CAS# 115733-08-9; Benzene C_{14}-C_{24} branched and linear alkyl derivatives • CAS# 68081-77-6; Benzene polypropene derivatives Arylpolyolefins are manufactured by mixing anhydrous alkylate (linear or branched) with benzene in the presence of catalyst and heat. More information on the Arylpolyolefin Category can be found in the American Chemistry Council; Petroleum Additives Panel; Health, Environmental, Regulatory, Task Group, High Production Volume test plan for this category (2). 2. Health, Environmental, Regulatory, Task Group (HERTG). 2002. High Production Volume (HPV) Chemical Challenge Program Test Plan For The Arylpolyolefin Category. American Chemistry Council, Petroleum Additives Panel, HERTG.
Conclusion:	Substances in the Arylpolyolefin Category are expected to distribute primarily to soil with a small percentage partitioning to sediment. These data represent a key study for characterizing the fugacity of the Arylpolyolefin Category, which includes benzene C_{14}-C_{24} alkyl derivatives (CAS # 115733-08-9)

	and benzene polypropene derivatives (CAS # 68081-77-6). Comparatively, their potentials to partition in the environment are expected to be similar, based on their high log Kow and low water solubility values.
Reliability:	(2) Reliable with restrictions The input data used to run the EQC Level I model include estimated values calculated by the EPIWIN program based on chemical structure. The partitioning data represent a potential distribution range for substances in the two CAS numbers listed under test substance. Computer modeling is an accepted method of assessing environmental distribution of chemicals.
Reference:	Mackay, D.A. DiGuardo, S. Paterson, and C. Cowan. EQC Model Version 1.01. 1997. Available from the Environmental Modeling Centre, Trent University, Canada.
Other (source):	American Chemistry Council; Petroleum Additives Panel; Health, Environmental, Regulatory, Task Group

* Other TS is an option in the "test substance" pick list within the IUCLID data entry field for "transport / distribution". Selecting this option refers the reader to information in the "freetext" field for "test substance".

4.1 Acute Toxicity

4.1.1 Acute Oral Toxicity

Robust Summary #: 2-Acute Oral-1

Test Substance	
CAS #	CAS# 115733-08-9
Chemical Name	Benzene C14-C24 alkyl derivatives
Remarks	Test material dosed as received, purity not provided.
Method	
Method/Guideline followed	FHSA 16CFR1500.3
Test Type	Acute oral toxicity
GLP (Y/N)	N
Year (Study Performed)	1978
Species/Strain	Rats/ Sprague-Dawley strain
Sex	Male/Female
No. of animals/dose	5/sex
Vehicle	Corn oil
Route of administration	Oral (intragastric)
Dose level	5 g/kg
Dose volume	10 ml/kg
Control group included	No
Remarks field for test conditions	A single dose of the test material was administered intragastrically to five fasted male and female rats at each treatment level. The animals were observed for signs of toxicity or behavioral changes during the 4 hours post dosing and daily thereafter. Individual weights were recorded on the day of dosing, on day 7 and at termination. All animals were euthanized at the conclusion of the observation period. Gross autopsies were performed on all animals after 14 days.
Results	LD50 > 5 g/kg (males and females)
Remarks	All animals survived the duration of the study. Two males and two females were hypoactive at 1 hour post dosing and two females exhibited urine staining of the fur at 4 hours post dosing. All animals exhibited progressive body weight gains at each weighing interval. At necropsy one male exhibited an enlarged spleen and one female exhibited hydrometra of the uterus.
Conclusions	The test article, when administered to male and female Sprague-Dawley rats, had an acute oral LD50 of >5 g/kg.
Data Quality	Reliable without restriction (Klimisch Code).
References	Unpublished confidential business information
Other	Updated: 1/21/02

Robust Summary #: 2-Acute Oral-2

Test Substance	
CAS #	CAS# 68081-77-6
Chemical Name	Benzene, polypropene derivatives
Remarks	Test material dosed as received, purity not provided.
Method	
Method/Guideline followed	43 CFR 37336, 163.81-1
Test Type	Acute oral toxicity
GLP (Y/N)	Y
Year (Study Performed)	1980
Species/Strain	Rats/Sprague-Dawley strain
Sex	Male/Female
No. of animals/dose	5/sex
Vehicle	None
Route of administration	Oral (intragastric)
Dose level	5g/kg
Dose volume	6.35 ml/kg
Control group included	No
Remarks field for test conditions	A single dose of the undiluted test material was administered intragastrically to ten fasted (over night) animals at a dose level of 5 g/kg. A control group was not included. The animals were observed for signs of toxicity or behavioral changes twice daily. Individual weights were recorded on the day of dosing and on days 7 and 14. All animals were euthanized at the conclusion of the observation period. Gross autopsies were performed on all animals after 14 days.
Results	LD50 >5g/kg (males and females)
Remarks	All of the treated animals survived the duration of the study. One male exhibited wheezing at 1 to 4 hours post dosing. Three males and all of the females exhibited urine soaked fur through day 1 on test. No other abnormal clinical signs were observed. All animals gained body weight during the study. No treatment related gross postmortem findings were evident at necropsy.
Conclusions	The test article, when administered as received to male and female Sprague-Dawley rats, had an acute oral LD50 >5g/kg.
Data Quality	Reliable without restriction (Klimisch Code)
References	Unpublished confidential business information
Other	Updated: 1/21/02

4.1.2 Acute Dermal Toxicity

Robust Summary #: 2-Acute Dermal-1

Test Substance	
CAS #	CAS# 115733-08-9
Chemical Name	Benzene C14-C24 alkyl derivatives
Remarks	Test material purity not provided
Method	
Method/Guideline followed	OECD Test Guideline 402
Test Type	Acute dermal toxicity (Limit Test)
GLP (Y/N)	Y
Year (Study Performed)	1980
Species/Strain	Rabbits/New Zealand White
Sex	Male and female
No. of animals/sex/group	5
Vehicle	None
Route of administration	Dermal
Dose level	2 g/kg
Dose volume	2.3 ml/kg
Control group included	No
Remarks field for test conditions	Approximately 24 hours prior to topical application of the test material, the hair of each animal was closely clipped. The skin was not abraded. A single dose of 2 g/kg of the undiluted test material was administered dermally to five male and female animals. The test material was kept in contact with the skin for a period of 24 consecutive hours under a surgical dressing and plastic film. The application site was wiped clean of residual test material at the end of the 24-hour exposure period using saline. The animals were observed frequently for clinical signs on the day of dosing and once daily for 14 days after treatment. Individual body weights were recorded on the day of dosing and on days 7 and 14. Gross necropsies were performed on all animals on Day 14
Results	LD50 > 2.0 g/kg (males and females)
Remarks	No mortality was observed. The mean body weight of the males increased slightly during the study. The mean body weight of the females was unchanged during the study. Dermal irritation (erythema and edema) was observed in all rabbits and persisted at least 4 days post dosing. No treatment related gross necropsy effects were evident.
Conclusions	The test article, when administered dermally as received to 5 male and 5 female New Zealand white rabbits had an acute dermal LD50 of greater than 2.0 g/kg.
Data Quality	Reliable without restriction (Klimisch Code).
References	Unpublished confidential business information
Other	Updated: 1/21/02

Robust Summary #: 2-Acute Dermal-2

Test Substance	
CAS #	CAS# 68081-77-6
Chemical Name	Benzene, polypropene derivatives
Remarks	Test material purity not provided
Method	
Method/Guideline followed	43 CFR 37336, 163.81-2
Test Type	Acute dermal toxicity (Limit Test)
GLP (Y/N)	Y
Year (Study Performed)	1980
Species/Strain	Rabbits/New Zealand White
Sex	Male and female
No. of animals/sex/group	5
Vehicle	None
Route of administration	Dermal
Dose level	2 g/kg
Dose volume	2.54 ml/kg
Control group included	No
Remarks field for test conditions	Approximately 24 hours prior to topical application of the test material, the hair of each animal was closely clipped. Immediately prior to dosing the skin was abraded. A single dose of 2 g/kg of the undiluted test material was administered dermally to five male and female animals. The test material was kept in contact with the skin for a period of 24 consecutive hours under an elastic bandage. The application site was wiped clean of residual test material at the end of the 24-hour exposure period. The animals were observed for abnormal clinical signs twice daily for 14 days after treatment. Skin condition was evaluated daily. Individual body weights were recorded on the day of dosing and on days 7 and 14. Gross necropsies were performed on all animals on Day 14
Results	LD50 > 2.0 g/kg (males and females)
Remarks	No mortality was observed. All animals gained weight during the study. No abnormal clinical signs were observed during the study. One male exhibited slight and moderate erythema and one female exhibited slight erythema during the study. These animals also exhibited desquamation. No treatment related gross necropsy effects other than skin effects were evident.
Conclusions	The test article, when administered dermally as received to 5 male and 5 female New Zealand white rabbits had an acute dermal LD50 of greater than 2.0 g/kg.
Data Quality	Reliable without restriction (Klimisch Code).
References	Unpublished confidential business information
Other	Updated: 1/21/02

5.0 Genetic Toxicity

Robust Summary #: 2-GenTox-1

Test Substance	
CAS #	CAS# 115733-08-9
Chemical Name	Benzene C14-C24 alkl derivatives
Remarks	Test material purity not provided.
Method	
Method/Guideline followed	OECD Guideline 471
Test Type	Bacterial Reverse Mutation Assay
GLP (Y/N)	Y
Year (Study Performed)	1981
Test System	**Salmonella typhimurium**
Strains Tested	*Salmonella typhimurium* tester strains TA98, TA100, TA1535, TA1537, TA1538
Exposure Method	Plate incorporation
Test Substance Doses/concentration levels	0.025, 0.075, 0.25, 0.75 and 2.5 mg/plate with and without activation
Metabolic Activation	With and without (S9 fraction mix of livers of Aroclor 1254 pretreated Sprague Dawley rats)
Vehicle	Ethyl acetate
Tester strain, activation status, Positive Controls and concentration level	TA98 +S9 2-aminoanthracene 5 ug/plate TA98 -S9 2-nitrofluorene 5 ug/plate TA100 +S9 2-aminoanthracene 5 ug/plate TA100 -S9 sodium azide 30 ug/plate TA1535 +S9 2-aminoanthracene 5 ug/plate TA1535 -S9 sodium azide 30 ug/plate TA1537 +S9 2-aminoanthracene 5 ug/plate TA1537 -S9 9-aminoacridine 10 ug/plate TA1538 +S9 2-aminoanthracene 5 ug/plate TA1538 -S9 2-nitrofluorene 5 ug/plate
Vehicle Control	Ethyl acetate
Statistical Analysis	Mean revertant colony count and standard deviation were determined for each dose point.
Dose Rangefinding Study	No
S9 Optimization Study	No
Remarks field for test conditions	This study was conducted prior to the development of OECD Guideline No. 471. This study deviates from the guideline in that Tester Strain TA 1538 is not called for in the guideline but it was included. In addition E. coli WP2 urvA Tester Strain called for in the guideline was not include. There were two treatment sets for each tester strain, with (+S9) and without (-S9) metabolic activation. Each of the tester strains was dosed with five concentrations of test substance, vehicle control, and a positive control. Three plates/dose

	group/strain/treatment set were evaluated. 50-100 ul of test material, positive control or vehicle control were added to each plate along with 100 ul of tester strain, S9 mix (if needed) and 2.0 ml of top agar. This was overlaid onto the surface of minimal bottom agar in a petri dish. Plates were incubated for 48 hours at 37°C. The numbers of revertant colonies were counted with an automated colony counter. The test material was considered a mutagen if a dose related increase was found in the number of revertant colonies and if the first dose level considered for the increase had an average number of revertant colonies that was three times that of the vehicle control.
Results	The test substance was not genotoxic in this assay with or without metabolic activation.
Remarks	All data were acceptable and no positive increases in the number of revertants/plate were observed with any of the tester strains with or without metabolic activation. The positive control for each respective test strain exhibited an appropriate response (with or without S9) over the mean value of the vehicle control for a given strain, confirming the expected positive control response.
Conclusions	Under the conditions of this study, the test material was not mutagenic.
Data Quality	Reliable with restriction (Klimisch Code). Restriction due to the lack of any information regarding the selection of dose levels used during the study. In addition no information is presented regarding cytotoxicity or the presence of test material precipitate in the cultures.
References	Unpublished confidential business information
Other	Updated: 10/24/2002